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ANNUAL REPORT
2008

SANDIA NATIONAL LABORATORIES

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Sandia National Laboratories

Abstract

Sandia National Laboratories has traditionally contracted for university research to expand its science and technology base to assure the performance of its nuclear weapons. Sandia and its strategic university partners are seizing the opportunity to establish enduring relationships that produce world-class joint R&D, educate next generation employees, provide Sandians with continuous learning opportunities, and develop national constituency and name recognition. Sandia's university research investments are made, for the most part, by individual technical programs. The University Research Programs Office serves as the point of contact for all university research issues and creates and implements those processes and tools that enable university partnerships. The office also manages several university-related programs (Campus Executive Program, Sandia University Research Program, and the Presidential Early Career Award for Scientists and Engineers), through which investments are made in students and faculty via contract research and graduate research projects. In addition, the University Research Programs Office, in partnership with Human Resources, oversees the President Harry S. Truman Fellowship in National Security Science and Engineering Program (Truman Fellowship) and programs that forge new strategic relationships in critical skills areas. The FY2008 University Research Annual Report details the projects supported by Sandia in these university-related partnerships programs.

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An Overview of Sandia National Laboratories' University Research Investments

Marie L. Garcia

The nation's investment in science has been in crisis for some time, especially in the physical and engineering sciences. Federal support for academic R&D began falling in 2005 for the first time in a quarter century, while Federal and industry support for their own basic research has stagnated over the last several years.[1] R&D investment from industry has not filled the gap, perhaps because industry views such investments as strongly slanted toward development, when application is a closer match to their shareholder-driven requirements. In addition to leading to a weakened technology base for both U.S. industry and the national defense enterprise, these declines in support set the stage for future challenges in attracting the scientific research talent we need in this critical area.

Our nation's business and academic leaders came together in 2005 to issue a series of reports that convincingly document the threats to continued U.S. economic primacy and, more important, offer an action agenda to address the many global challenges facing our country today. In particular, the National Academies released a report, Rising Above the Gathering Storm, which reinforces an urgent message: if trends in U.S. research and education continue, our nation will squander its economic leadership, and the result will be a lower standard of living for the American people.

Many other countries are pouring money into building their science and technology enterprises. In fact, many of these countries are emulating our innovation model-leveraging investment in science and technology to create market leadership—with remarkable success. America's leaders and its citizens have traditionally pursued policies that encouraged innovation by funding Federal investment in basic research, improving education at all levels, allowing the U.S. to attract the best and the brightest from around the world. Today, we must follow those footsteps and take the actions necessary to keep the U.S. at the forefront of an increasingly competitive global economy. Partnerships with universities, industry, and other national laboratories are essential to address this issue.

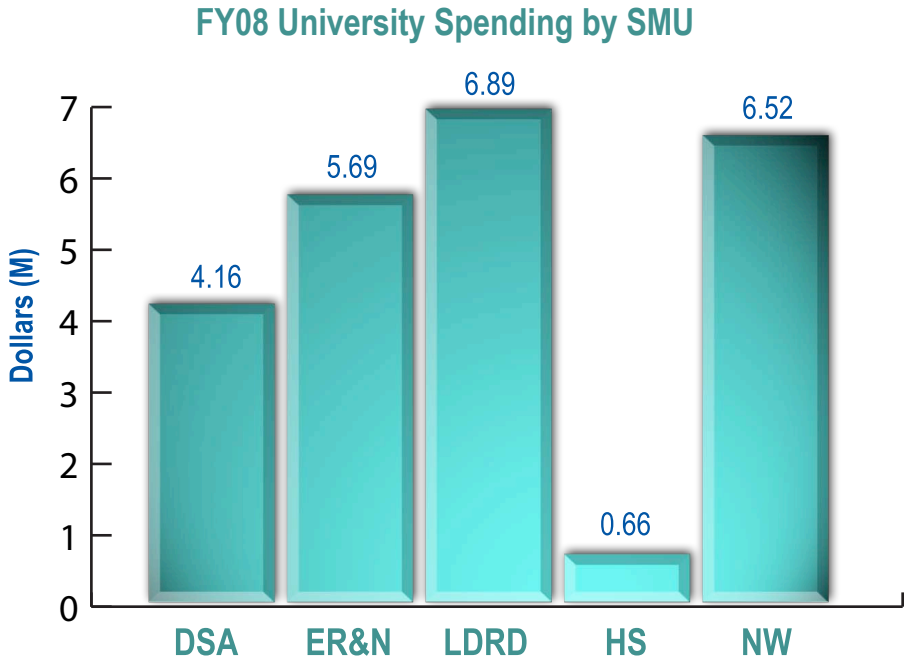

Figure 1. Sandia investments in university research in FY08, by Strategic Business Units[2]

For over fifty years, Sandia National Laboratories (Sandia) has focused on being the laboratory that the U.S. turns to first for technology solutions to the most challenging problems that threaten peace and freedom for the nation and the globe. University partnerships have been and will continue to be a critical element in achieving this goal. Sandia has traditionally contracted for university research to expand its science and technology base to assure the performance of its nuclear weapons.

Sandia and its strategic university partners are seizing the opportunity to establish deeper, enduring relationships that produce world-class joint R&D, educate next generation employees, provide Sandians with continuous learning opportunities, and build national visibility and name recognition. In FY2008, Sandia invested approximately $24 million in 491 joint research projects with 93 universities (Figure 1) in five mission-related areas. FY08 research investments are down from $24.7m in FY07. Despite reduced budgets and a recessive economy, Sandia's investment in university research continues at a steady state. The research projects reported in the following pages represent only the corporate investment portion of Sandia's total investment in research collaborations. Sandia invests additional

[1]National Science Foundation, National Science Board, Science & Engineering Indicators 2008, p.1
[2]Defense Systems & Assessments (DSA), Energy, Resources & Nonproliferation (ER&N), Laboratory Directed Research and Development (LDRD), Homeland Security (HS), Nuclear Weapons (NW)

monies for graduate student support, tuition assistance for employees, and university and K-12 science outreach. The strategic partnerships of the future will be additionally be directed towards those joint activities that will help ensure national competitiveness in the twenty-first century.

The University Research Programs Office provides the leadership and framework for execution of the Laboratories' university partnerships strategy, as well as leadership within the Nuclear Weapons Complex regarding the role of university partnerships in supporting Complex Transformation. The Programs Office executes this strategy primarily through management of the Campus Executive Program, the umbrella under which corporate investments in research, recruiting and education are aligned with the Campus Executive universities. The Programs Office also manages several other university-related programs including the Graduate Research Program, Sandia University Research Program, Presidential Early Career Award for Scientists and Engineers, and the Truman Fellowship. Through these programs, investments are made in students and faculty via contract research and graduate research projects. These investments are intended to help accelerate the creation of world-class research, produce future generations of scientists and engineers, and grow competencies and new businesses for Sandia.

The Programs Office serves as the point of contact for university research issues and develops and implements those tools and processes that enable university partnerships. One major area of emphasis includes further development of the partnership between Sandia and the University of Texas System (UTS). The overarching goal is to achieve a greater mutual impact on national security issues. Its strategic purpose is to participate with Sandia scientists on collaborative research projects, to provide peer review for Sandia's research programs, and to provide specialized courses taught by UTS professors to increase educational opportunities for Sandians.

In FY2008, the President Harry S. Truman Fellowship in National Security Science and Engineering Program (Truman Fellowship) entered its fifth year. This program provides an opportunity each year for exceptional scholars to join Sandia in the continuation of Sandia's tradition of excellence. Two new Truman Fellows joined Sandia in 2008. They came from the University of Arizona and the Swiss Federal Institute of Technology.

Investments in university research continue to pay off handsomely for Sandia and for U.S. taxpayers. This University Research Annual Report showcases the excellent results of these investments. Our joint accomplishments can be measured by the number of journal articles published, patents and copyrights issued, new collaborations, and new employees hired. New collaborations through the Sandia-University Research Program (SURP) include the National Science Foundation (NSF), the National Institutes of Health, the Mental Illness and Neuroscience Discovery (MIND) Institute, the University of Connecticut, and Arizona State University. A User Agreement was approved at the Center for Integrated Nanotechnologies (CINT), a DOE/Office of Science research center that operates as a national user facility devoted to establishing the scientific principles that govern the design, performance, and integration of nanoscale materials. Collaborations forged through the Graduate Research Program include NSF's Science and Technology Center for the Sustainability of Semi-Arid Hydrology and Riparian Areas (SAHRA) and the Pima County Flood Control District; and, a separate partnership with the National Aeronautics and Space Administration regarding Fourier analysis and synthesis tomography (FAST).

As a national laboratory, Sandia is proud to continue on the path established by Vannevar Bush, science advisor to Presidents Franklin D. Roosevelt and Harry S. Truman, who asserted that the Federal government should facilitate science and technology by funding researchers in the nation's universities and national laboratories, and by supporting the training of the next generation of scientists. Bush's advice to President Roosevelt became the seminal study, Science: The Endless Frontier, issued by the Executive Office of Scientific Research and Development in 1945, and led to the establishment of the National Science Foundation in 1950.

CAMPUS EXECUTIVE PROGRAM

Sandia National Laboratories (Sandia) has as its highest goal to become the laboratory that the U.S. turns to first for technology solutions to the most challenging problems that threaten peace and freedom for the nation and the globe. University partnerships are a critical element in achieving this goal. Sandia has traditionally contracted for university research to expand its science and technology base to assure the performance of its nuclear weapons. Opportunities exist beyond this status quo. Both Sandia and universities share a need to accelerate the creation of world-class research, produce scientists and engineers, and grow competencies and new businesses. Today, Sandia partners with key universities to achieve three major objectives: conduct world-class science, hire world-class scientists and engineers, and develop strategic collaborations in focused research areas.

The Sandia Campus Executive Program was established in 1997 as a means to help accomplish these objectives. It provides a framework for Sandia to focus its research goals and helps create the 21st century workforce needed to perform the technical jobs crucial to fulfilling its national security mission. Sandia executives, acting in the role of ambassadors, are paired with top university officials (usually vice presidents of research and/or deans of engineering) at schools that have synergistic research interests and capabilities with Sandia. These Sandia executives are tasked with the responsibility of working with the universities to implement programs established for the express purpose of furthering the goals of both Sandia and the universities.

This program encourages the Campus Executives to work with their university counterparts to develop and implement action plans that satisfy the needs of each institution. They employ an integrated investment approach whereby research, talent, and advocacy needs are worked simultaneously, not independently. The Campus Executives schedule visits to their assigned universities once or twice each year, serve on university advisory boards, and attend special events. They interface with campus recruiting teams to actively support placing students in the numerous Sandia programs. The Campus Executives also interface with university faculty to promote sabbaticals, placements, and exchanges. This program enables the Campus Executives to deliver a coordinated message to educate key university personnel regarding the infrastructure and programs being put in place to mutually benefit both Sandia and its strategic university partners. In 2008, 21 universities were considered the corporate key/regional universities with which campus executives interacted.

Each Campus Executive has $50k/year of Laboratory Directed Research and Development (LDRD) funding earmarked for investments in either graduate research projects or contract research at their university. Based on the plan developed for each university, the Campus Executive determines the appropriate investment of that money. At some schools, the Campus Executive, working with the deans of engineering or arts and sciences, may employ the strategy of establishing graduate research projects for doctoral students doing research in areas in which the Labs has an interest. In these instances, the student and a Sandia Principal Investigator are matched to identify a research project and conduct the research. In many cases, the Sandia Principal Investigator or the Campus Executive becomes a member of the student's doctoral committee. With the Sandian on the doctoral committee, the Labs not only builds relationships with other professors but also is able to offer direct input in the research direction. The desired result of these research projects is to develop a long-term relationship with students that show promise of becoming future Sandia employees, educated and trained in areas of importance to Sandia. At other universities, the Campus Executive elects to invest his/her money in a research project as a means to "seed" an area that looks promising, with the strategy of Sandia and the university eventually collaborating for third-party funding.

For 2008, the following were the Campus Executive/University assignments.

University	Campus Executive	Deputy Campus Executive	Research Focus Area
Caltech	Gerry Yonas	Tim Shepodd	Cognitive Neuroscience
Carnegie Mellon	Vacant	Larry Shipers	Computer Science/Robotics
Cornell	Gerry Yonas	Jonathan Custer	Cognitive Neuroscience
Georgia Tech	Jill Hruby	Dave Womble	Microsystems Research
MIT	Jim Woodard	Gerry Sleefe	Infrastructure Surety
New Mexico State University	Steve Rottler	Anthony Medina	Water Research
New Mexico Tech	Jim Chavez	Paul Shoemaker	Explosives/Energetic Materials
Purdue	Joe Polito	Marcey Abate	Nanotechnologies & Microsystems Res
Stanford	Joan Woodard	Glenn Kubiak	Materials Mechanics Modeling
Texas A&M University	Les Shephard	James Peery	Global Nuclear Security
University of Arizona	Duane Dimos	Ray Finley	Water Systems Modeling
University of California at Berkeley	Terry Michalske	Blake Simmons	Microsystems Research/Energy
University of California at Davis	Len Napolitano	Mike Hardwick	Info Security/Embedded Reasoning
University of Colorado at Boulder	David Plummer	TBD	Microsystems Research
University of Florida	Tom Hunter	Regan Stinnett	Micro/Nano Science & Engineering
University of Illinois at Urbana-Champaign	Dave Carlson	Russ Skocypec	Nano Science/Cognitive Neuroscience
University of Michigan	Bob Carling	Brandon Levey	Microsystems Research
University of New Mexico	Rick Stulen	Rob Leland	Nano Science & Engineering/ModSim
University of Texas at Austin	Jerry McDowell	Art Ratzel	Nano Science & Engineering
University of Texas at El Paso	Gil Herrera	Ernest Garcia	Advanced Manufacturing
University of Wisconsin	John Stichman	Mark S. Allen	Nuclear Eng/Computational Sciences

Neural Correlates of Attention and Intention in Decision-making of Macaques and Humans: Selective Lesioning of Posterior Parietal Areas during Electrophysiology and fMRI

Tamara Knutsen
California Institute of Technology

Tim Shepodd (Org. 8223)
Sandia Principal Investigator

Project Purpose

The purpose of this work with the California Institute of Technology (Caltech) is to discover the specific relationships (spatial and temporal) between decisions and actions of the brain. In vivo (macaque) visualization of perception, motivation, and decision will take place aided by reversible cortical lesioning. GABAa (Gamma-amino butyric acid receptor "a") agonists inactivate either the parietal reach region or the lateral intraparietal area (LIP) while the other region is monitored with electrophysiological recording and functional magnetic resonance imaging (fMRI).

Accomplishments

A map of the cortical region within the chamber implant has been constructed by sampling electrode placements with one millimeter spacing and recording neuronal activity during a standard saccade and reaching task. Spike tuning of the neurons for intended movement direction for either eye or arm effector was assessed, in real time, with custom Matlab code. These results were re-confirmed with offline sorting software. This observed data was compared to the high-resolution magnetic resonance imaging (MRI) data to ensure that functional areas are within expected anatomical bounds and to plan the optimal injection location. An injectrode, a modification of a prototype described in the literature, was built to integrate into the NAN recording drive so multiple physiological locations can be monitored during inactivation. This approach provides multiple benefits, including confirmation that injected area is silenced, confirmation that surrounding functional areas are unaffected by GABAa agonists, by verifying maintenance of normal firing rates, and the ability to assess any changes in neuronal tuning properties in nearby areas due to the lack of input from the silenced area. Protocol was amended to include the use of THIP (4,5,6,7-tetrahydroisoxazolo-[5,4-c]-pyridin-3-ol) a rigid, bicyclic isoxazole derivative of GABA that has recently been distinguished from GABA and muscimol by virtue of its greater relative specificity.

Significance

Understanding how the brain functions is key to mapping the stages of decision-making in the brain. The relationships among stimulus, perception, decision, and action allow the thought process to be understood in fantastic detail. This has national security implications and is valuable to future systems that could control artificial limbs.

Improving Robot Navigation Through Self-supervised Online Learning

Boris Sofman
Carnegie Mellon University

Charles Little (Org. 6473)
Sandia Principal Investigator

Project Purpose

This project with Carnegie Mellon University explores how self-supervised online learning techniques can be applied to robotics, particularly autonomous outdoor navigation, in order to allow robotic systems to improve their performance over time. If an autonomous system can learn, online, the capabilities of autonomous and tele-operation control and identify the situations in which they tend to struggle, then it can maximize autonomous operation, while using the human where intervention is most required. This can then be incorporated into the robot planner to avoid areas that would require heavy human involvement. In the end, one operator can then oversee the performance of many robots.

Accomplishments

We were able to make significant progress on developing a framework for the assisted autonomy setting. We developed a k-bandits–based framework for modeling the tradeoff between exploration and exploitation of knowledge in such a setting. We were also able to make significant progress on developing a novelty detection system to allow a robot to identify situations that have not been previously encountered and therefore are potentially high-risk and require human oversight. By reducing the dimensionality of the high-dimensional features from the perception system or overhead data, we were able to use a form of density estimation to identify areas of the feature space that represent potentially novel situations with respect to previously seen data. We plan to submit this portion of the work to the International Conference on Robotics and Automation and continue development and on-board testing of the full assisted autonomy system.

Significance

Autonomous robot navigation is a critical technology for several Sandia mission areas. These include

nonproliferation and assessments, military technologies and applications, and homeland security. Under nonproliferation and assessments, autonomous robot technology can be used to aid robots performing site assessments. Similarly, there are many military applications for autonomous robots. For homeland security, robots are used in a wide range of activities that include emergency response and physical security. The autonomous navigation technologies developed under this project will enhance robot performance for this wide range of applications.

Physiological Models and Inference Based on Optical Imaging

Nathan Cornelius
Cornell University

Carl Diegert (Org. 1412)
Sandia Principal Investigator

Project Purpose

The purpose of the project with the Weill Cornell Medical College of Cornell University is to develop mathematical models, and video processing based on the models, that relate electrical activity of the brain to video optical reflectance spectroscopy data. Since the spectroscopy data is directly related to the amount of hemoglobin present in each pixel of brain tissue and whether it is oxygenated or deoxygenated, the model is basically a description of the neurovascular response of the brain. The immediate focus is on epilepsy, but other neurological conditions can also be examined through the same neurovascular response.

Accomplishments

We have developed a complete mathematical model of the neurovascular response and the optical measurements. The model has multiple layers that interact: electrical, metabolic, vascular, and optical. Each layer tries to incorporate relevant physiology, within the limits of the data. For example, the data is really surface data, so there is no third dimension of depth into the cortex of the brain, and the pixels of the data are too large to permit visualization of individual neurons, let alone neuronal processes. The model can be presented in two forms: as a 2D array of interconnected ordinary differential equation models at each pixel or as a partial differential equation. While the pixel version is directly comparable to the pixel data, the partial differential equation allows analytical solution of the model for idealized inputs and idealized tissue parameter geometries, which is very helpful in understanding the behavior of the nonlinear model. The last conceived, and probably the most unusual, aspect of this model is the representation of the vascular layer as an electric circuit with two "charge carriers," oxygenated and deoxygenated hemoglobin, which is parametrically excited by the metabolic layer. In parallel, we have pursued video processing of the experimental data to normalize the data and improve its signal-to-noise ratio.

Significance

The key aspect of the model is that it is very flexible, while at the same time, having a limited number of parameters, each of which has a physiological interpretation. For instance, a small volume of brain tissue can be perfused directly from an arterial source, from neighboring volumes of brain tissue, or from a mixture. Therefore there we expect to be able to estimate the parameters from data, and then, with two different sets of data, be able to estimate two different sets of parameters and make meaningful statements about whether there is a functional difference.

Advances from this project will enable better fusion of data from various modalities and more precise physiological models of the brain that will be useful for national security applications such as treatment and prevention of post-traumatic stress disorder (PTSD) and traumatic brain injury, advances in lie detection and intent detection, and classifying and improving human performance in critical tasks (e.g., decision-making under high stress).

Advanced I/O for Large-scale Scientific Applications

Jay Lofstead
Georgia Institute of Technology

Ron Oldfield (Org. 1422)
Sandia Principal Investigator

Project Purpose

The purpose of this work is to develop a mechanism by which high performance computing (HPC) applications can employ high-performance, metadata-rich input-output (I/O) that is adaptable without source code changes to whatever mechanism provides the best performance for each I/O operation for the selected platform and scale. As part of the I/O operation, insertion of low-impact, application-specific data annotation and transformation operations are included to enhance scientist productivity. This project represents a collaboration with the Georgia Institute of Technology.

Accomplishments

We identified the following basic issues related to decomposition of data transformations into discrete operations.

- The granularity and richness of operations may affect optimization opportunities. While richer operations require fewer transforms, more-granular operations provide more-explicit opportunities for optimization.
- It is unclear whether it is better to combine identical operations or duplicate them.
- As clients are added and removed for a file stream, at what performance degradation level is it worth redeploying the overlay network? How can that be calculated?

We designed and evaluated techniques for creating dynamic type and transformation information based on incoming data type, outgoing data type, downstream transformation requirements, and transformation operations.

We explored techniques for the distribution of transformation operations in the presence of various restrictions on the system, and we designed and implemented two deployment schemes that change the organization of the transformations based on data size and end-to-end performance.

We analyzed the different types of I/O performed by the following parallel codes: GTC, GTC_S, Chimera, and XGC1 to determine a simple application programming interface (API) for a number of different I/O operations.

We designed and developed the asynchronous input-output (AI/O) API called ADIOS and demonstrated the efficacy of the system by replacing all of the I/O in the above parallel codes with our new API calls.

We tested application benchmarks using POSIX I/O, MPI Collective I/O, and our asynchronous methods.

We consulted with the climate groups at the National Center for Atmospheric Research (NCAR), Pacific Northwest National Laboratory (PNNL), and the National Aeronautics and Space Administration (NASA) to understand their performance concerns regarding our I/O techniques.

We developed an intermediate file format optimized for write performance while still maintaining conversion compatibility with HDF-5 (hierarchical data format-5) and NetCDF (network common data form).

We developed the idea of data characteristics to give a low-impact way to get a sense of science data without full data-indexing techniques.

Significance

The ADIOS API and associated technologies provide an easy-to-use API with the adaptability required to change I/O for science codes to use methods providing the best performance for the platform and scale used. By changing the I/O approach without changing the source code, scientists can more quickly and easily change the I/O methods employed to avoid poorly performing I/O methods on particular hardware. The additional metadata provides scientists with sufficient information to identify likely data sets for analysis without having to read and parse the entire data set.

Passive High-flux Thermal Management of Electrochemical Systems with *in situ* Microchannel Phase Change

Todd Bandhauer
Georgia Institute of Technology

Mike Kanouff (Org. 8365)
Sandia Principal Investigator

Project Purpose

Energy-storing electrochemical batteries are the most critical components of hybrid and electric vehicles. Lithium-ion batteries are proposed to improve the fuel economy of these vehicles because of their higher specific energy, but face thermal management challenges. Thermal management to maintain a specific operating temperature window of individual cells and packs is essential to maintain the performance of these batteries. This research with the Georgia Institute of Technology addresses the singular limiting feature of battery cooling systems — the cooling systems are external to the batteries, which implies that substantial temperature gradients exist between the heat generation location (the cells) and the skin of the battery.

Accomplishments

We conducted a comprehensive review of the literature relevant to thermal issues in lithium-ion batteries, which revealed significant gaps in the understanding of heat generation and transport mechanisms within these batteries. This work has been prepared as a critical review paper submission to an archival electrochemical publication. In addition, we developed a one-of-a-kind, two-dimensional thermal model for a flat, spirally wound lithium-ion battery. Using findings from the literature review, the model accounts

for heat transport inside the battery for variable rates of heat generation throughout discharge. The model is able to account for spatial variations within the battery at high resolution, temporal variations in transfer rates, and also, a variety of heat generation mechanisms. This work was presented at an Electrochemical Society conference in Fall 2008. Predictions of temperature profiles with a variety of imposed heat generation rates, thermal resistances, and cooling mechanisms have been made to understand the influences of the governing influences on internal battery temperatures. We have also simulated a battery with the proposed embedded microchannel heat transfer solution, yielding predictions of substantial improvement in cooling capacities and internal battery temperatures compared to all other externally cooled thermal management systems.

Significance

The models developed could be used to design, fabricate and test a representative battery cooling system. The minimization of peak temperatures and gradients within batteries will allow increased power and energy densities unencumbered by thermal limitations. These storage devices will also see application in the spatial and temporal concentration of renewable energy sources and in the harvesting of low-grade energy. Discussions have been held with: a) other collaborators for assistance in fabrication issues, b) several battery manufacturers who have expressed a strong interest in the proposed thermal management concept, and c) with major automotive manufacturers who have also confirmed the need for such a system.

Effect of Pressure and Particle Size on Microstructure and Properties of Vacuum-Plasma-Sprayed Yttria-Stabilized-Zirconia Solid Oxide Fuel Cell Electrolytes

Nick Spinhirne
New Mexico Institute of Mining and Technology

Aaron Hall (Org. 1813)
Sandia Principal Investigator

Project Purpose

The purpose of this project with the New Mexico Institute of Mining and Technology (New Mexico Tech) was to improve our understanding of low-pressure plasma-spray thin-film (LPPS-TF) processing of yttria-stabilized zirconia (YSZ) coatings for use as solid oxide fuel cell (SOFC) electrolytes.

Accomplishments

During this project, we became the second facility in the world to successfully demonstrate the ability to prepare columnar YSZ coatings using the LPPS-TF process. In addition, we prepared YSZ coatings with lamellar, and mixed (lamellar and columnar) microstructures. Electrical properties of these coatings relevant to SOFC electrolytes were measured at New Mexico Tech.

Significance

This work has advanced our understanding of the LPPS-TF process and has demonstrated that it can be used to create unique microstructures in YSZ coatings. This knowledge will allow us to more easily use LPPS-TF to prepare coatings with other ceramic materials.

Micro-rheology of Polymeric Materials at High Strain Rates

Taylor Dotson
New Mexico Institute of Mining and Technology

Doug Adolf (Org. 1821)
Sandia Principal Investigator

Project Purpose

This project with the New Mexico Institute of Mining and Technology (New Mexico Tech) provides insight into the molecular mobility of polymers to be used as input to continuum, nonlinear viscoelastic, constitutive equations that allow engineers to model yield, creep, and physical aging of glassy polymers. Our current continuum model assumes that all relaxation modes available to a polymer scale with environmental conditions (e.g., temperature) in the same way, leading to the idea of a "material clock" that controls mobility. The model also assumes the clock depends on the potential energy of the system. Certain features of these assumptions were previously validated, but the current study examines these in more detail.

Accomplishments

Our previous, molecular dynamics studies of bead-spring chains demonstrated that the average mobility, as measured by the chain diffusion coefficient, was a unique function of the system potential energy, thereby validating a fundamental postulate of our continuum constitutive equation. However, relaxation functions offer an opportunity to examine these postulates more closely. A simple relaxation function tracks the correlation of the chain's end-to-end vector in time. We monitored this function for three types of chains: freely jointed (simple bead-springs),

freely rotating (adding in a bond angle), and torsional (adding in a torsional potential for the bond as well as the linear spring). Far from the glass transition, the shape of the relaxation functions for all systems did not change with environmental condition, in agreement with the "material clock" hypothesis. However, near the glass transition, the shape of the curves (monitored by the exponent in a Williams-Watt functional fit) changed, indicating a violation of this premise. Experimental systems also indicate such behavior for polymers deep in the glassy region, so these results do agree with data. Fortunately, the magnitude of change is not great, allowing one to still use this simplifying assumption in the continuum models. Indeed, the continuum models have been shown to accurately predict a broad range of responses for glassy epoxies.

Significance

The Sandia continuum constitutive equation for predicting glassy polymer response is the only current model that has been experimentally validated. With that validation, it has been used within our finite element codes to solve numerous practical problems. Therefore, understanding its fundamental postulates and perhaps uncovering possible improvements would benefit Sandia components. The model has been distributed to both industrial and academic partners.

Refereed Publications

T.C. Dotson, J.V. Heffernan, J. Budzien, K.T. Dotson, F. Avila, D.T. Limmer, D.T. McCoy, J.D. McCoy, and D.B. Adolf, "Rheological Complexity in Simple Chain Models," *The Journal of Chemical Physics*, vol. 128, p. 184905, May 2008

Improved Numerical Methods for Modeling River–Aquifer Interaction

Suzanne Tillery
New Mexico State University

Vince Tidwell (Org. 6313)
Sandia Principal Investigator

Project Purpose

The purpose of this research with New Mexico State University was to modify the MODFLOW-LGR software to allow local time-stepping for a "child" model, while simulating the "parent" model at the global time-interval. This allows the child model simulation time-interval to be smaller than the parent model time-interval, in order to capture transient events in areas with strong hydraulic variability, while leaving the coarser grid parent model at a larger time-interval that is appropriate in regions of minimal hydraulic variability. The MODFLOW series of software developed by the United States Geological Survey is generally accepted as the *de facto* industry standard for groundwater modeling.

Accomplishments

A new option for local time-stepping (LTS) was developed for use in conjunction with the multiple-refined-area grid capability of MODFLOW-LGR (MF-LGR). The LTS option allows each local, refined-area grid to simulate multiple stress periods within each stress period of a coarser, regional grid. The MF-LGR method for simulating multiple-refined grids essentially defines each grid as a complete model, then for each coarse grid time-step, iteratively runs each model until the head and flux changes at the interfacing boundaries of the models are less than some specified tolerances.

Use of the LTS option is illustrated in two hypothetical test cases consisting of a dual well pumping system and a hydraulically connected stream-aquifer system, and one field application. Each of the hypothetical test cases was simulated with multiple scenarios including an LTS scenario, which combined a monthly stress period for a coarse grid model with a daily stress period for a refined grid model. The other scenarios simulated various combinations of grid spacing and temporal refinement using standard MODFLOW model constructs. The field application simulated an irrigated corridor along the Lower Rio Grande River in New Mexico, with refinement of a small agricultural area.

The results from the LTS scenarios for the hypothetical test cases closely replicated the results from the true scenarios in the refined areas of interest. The head errors of the LTS scenarios were much smaller than from the other scenarios in relation to the true solution, and the run times for the LTS models were three to six times faster than the true models for the dual well and stream-aquifer test cases, respectively. The results of the field application show that better estimates of daily stream leakage can be made with the LTS simulation, thereby improving the efficiency of daily operations for an agricultural irrigation system.

Significance

Water scarcity has the potential to undermine the nation's energy, agricultural, and economic security. This work focuses on developing tools to better manage our limited resources.

Quite often, the surface water and groundwater equations for a coupled system are solved at the same time-step. However, in the vicinity of a strong stream-aquifer interaction, a small time-step is required to simulate

the interactions properly, while at distance in the aquifer, a much larger time-step may be adequate to accurately simulate the groundwater flow. Adding local time-stepping to a locally refined grid model has the advantage of maintaining solution accuracy while reducing simulation run time. Toward this need a modular local-time stepping package has been developed for the widely used groundwater-modeling package MODFLOW.

Tunnel Gap Modulation Spectroscopy: An Ultrasensitive Technique for Measuring Small Mass Change

Laura Biedermann
Purdue University

Steve Howell (Org. 1748)
Sandia Principal Investigator

Project Purpose

This project with Purdue University explored the feasibility of using multi-walled carbon nanotubes (MWNTs) as ultrasensitive mass sensors. The thermal oscillations of MWNTs under ambient conditions were measured using laser Doppler vibrometry (LDV). The high-frequency resolution of LDV enables a precise determination of the resonant frequencies and quality factors of the different eigenmodes of an oscillating MWNT. LDV is promising for automated detection because the predominant noise in the measured oscillation spectra is a low-power white noise background, which is clearly distinguishable from the optically reflected signal from the oscillating MWNT.

Accomplishments

To investigate the sensor properties of multi-walled carbon nanotubes (MWNTs), we explored the capabilities of laser Doppler vibrometry (LDV) to measure the thermal oscillation spectra of MWNTs. LDV uses the Doppler shift of a laser beam reflected from an oscillating object to measure that object's vibrational velocity. We also used Mie scattering theory to calculate scattering efficiency for MWNTs and developed a technique to add a gold-coated glass bead to individual MWNTs to extend the LDV technique to MWNTs with smaller diameters. The LDV technique seems applicable to any nanowire of interest and has already been used to measure the oscillation spectra of silver gallium nanowires.

The sharpness of the different oscillating resonant modes of a CNT is of high interest. We measured the quality factors of the resonance peaks. Subsequent calculations showed that air damping at atmospheric pressure is considerable for nanowires.

Furthermore, the LDV technique allowed reliable estimates for the Young's modulus of individual MWNTs. The LDV technique has the capability of providing accurate measurements of Young's modulus for a wide variety of nanowires. We also measured the Young's modulus of silver gallium nanowires provided by the University of Louisville.

An overview of the measurements of MWNT vibration spectra was presented at the 2008 March American Physical Society (APS) meeting and a manuscript summarizing this work has been submitted to *Nanotechnology*.

To enable measurements of the oscillation spectra of MWNTs under various atmospheres and pressures, we built a reduced atmosphere system capable of reaching pressures of 50 mTorr.

Significance

In order to increase the sensitivity of cantilevered microsensors and nanosensors, the mass of the cantilever needs to be decreased. MWNTs are ideal cantilevered nanosensors due to their small mass (~ 1 picogram). Even the smallest amount of analyte bonded to a MWNT will cause a detectable shift in the MWNT's oscillation frequency. Basic research into methods of measuring oscillation spectra with high frequency resolution is needed for MWNT sensor development. MWNTs, or a reflective bead affixed to the MWNT, could then be functionalized for use as nanoscale chemical and biological sensors.

Optical Properties of Plasmonic Metal-dielectric Composites

Mark Thoreson
Purdue University

Michael Pack (Org. 1128)
Sandia Principal Investigator

Project Purpose

The purpose of this project with Purdue University is to discover the optical properties of semicontinous silver film metamaterials, and use these materials in superlensing applications.

Accomplishments

We have studied the nanostructure and optical properties of semicontinuous silver films in the mid-infrared (IR) frequency range. These films can be tailored for use as mid-IR obscurants or filters. We have shown that film extinction spectra can be tailored by carefully adjusting the deposition conditions during film fabrication.

Our results on the photomodification of planar, semicontinuous metal films with picosecond pulses at

10.6 µm show both polarization- and wavelength-selective changes in the extinction spectra of the films.

Using images from experimental samples, we created distribution models, which were used as input in finite-difference time-domain (FDTD) simulations to predict far-field spectral responses. Using this technique, we are better able to predict the result of an experimental prototype and help direct subsequent fabrication processes more efficiently, by avoiding samples that are not suitable for the project's goals. Our simulations of the far-field spectra of realistic film geometries provide reasonable matching with the experimental spectral data.

We have obtained some interesting results related to the design, fabrication, and characterization of near-field superlens (NFSL) prototypes using a multilayer fabrication technique. A range of prototype samples were fabricated and characterized in order to study the effect of various parameters on the final NFSL prototype properties. Characterization included scanning electron microscopy, atomic force microscopy, far-field UV/Vis/NIR spectroscopy, and other techniques.

Significance

The ultimate goal of our work is the combination of the enhancement and superlensing aspects of composite films into a single system, allowing remote, enhanced sensing of analytes. This would enable the powerful sensing technique of surface enhanced Raman spectroscopy (SERS) to be used on materials that are currently impossible to sense with SERS.

Heat Conduction and Particle Motion in Stationary Nanofluids

Patricia Gharagozloo
Stanford University

Jonathan Zimmerman (Org. 8246)
Sandia Principal Investigator

Project Purpose

Nanofluids, nanoscale particles suspended in fluids, have been studied over the last decade for applications ranging from fluidic cooling to lubrication. Much of the research found thermal conductivity enhancements greater than predictions by effective medium theory, at low volume concentrations. However, large variations in data and dependencies have been observed. The goal of our measurements is to show how these variations can occur due to particle thermal diffusion away from the heated portion of the fluid and particle aggregation over time, by measuring the full field temperature and thermal conductivity distribution of nanofluids in a temperature gradient over time. This project is in collaboration with Stanford University.

Accomplishments

Initial light transmission measurements of 3% by volume (vol) alumina/boehmite nanofluid show thermodiffusion with decreasing intensity on the cold side and increasing intensity on the hot side. Thermal conductivity measurements of low stability 1% vol alumina nanofluids show a decrease in thermal conductivity, over time, corresponding to particle settling, over time. Thermal measurements conducted for stable 1%, 3%, and 5% vol alumina/boehmite nanofluids show conductivities initially at effective medium theory predictions. Over time, the 1% nanofluid remains within the experimental uncertainty preventing definitive conclusions regarding temporal variations. The 3% nanofluid shows large increases in conductivity on the cold side and small increases on the hot side, with an average increase of 20% after an hour. The 5% nanofluid shows a large temporal increase in conductivity of 30% throughout the nanofluid after an hour. The higher concentration nanofluids aggregate creating percolation paths over the aggregate. Models from percolation theory are consistent with the results. In the 3%, this effect is mainly on the cold side due to higher concentration levels from thermodiffusion. In the 5%, the concentration levels are high across the entire gap.

Initial light scattering measurements of aggregates in the 5% vol nanofluid show low fractal dimensions (less compact aggregates), which correspond to percolation theory predicting large increases in conductivity with aggregation. We have completed an initial model, modeling thermal conductivities based on particle material, aggregation, thermodiffusion, concentration, and boundary resistance between fluid and particle. We have developed a Monte Carlo simulation to model thermodiffusion, taking into account particle size distributions within the nanofluids. We have used this simulation to verify the initial concentration measurements and that the direct dependence of heat flux on particle mass flux from thermodiffusion is negligible. The Soret coefficient in the particle flux equation has been approximated as ~0.02 1/K, to be used in future modeling.

Significance

These measurements improve the understanding of nanofluid behavior due to particle diffusion and aggregation and show the importance of taking these effects into

account. They provide insights into how nanofluids may act in practical applications including microscale heat exchangers. A full understanding of nanofluids allows for determination of the usefulness of nanofluids to replace currently used fluids. These experiments also provide insights into the evolution of certain types of nanofluids, over time, showing how some degrade and others improve, over time. These results show that proper selection of nanofluids is important when considering their use in these applications.

Refereed Publications

P.E. Gharagozloo, J.K. Eaton, and K.E. Goodson, "Diffusion, Aggregation, and the Thermal Conductivity of Nanofluids," *Applied Physics Letters*, vol. 93, p. 103110, September 2008

Application of Advanced Laser Diagnostics to Hypersonic Wind Tunnels and Combustion Systems

Andrea Hsu
Texas A&M University

Jonathan Frank (Org. 8351)
Sandia Principal Investigator

Project Purpose

The purpose of this project with Texas A&M University is to conduct experimental research on non-equilibrium phenomena in hypersonic flows. The project is a fundamental study of supersonic combustion ramjet (SCRAMJET) propulsion and includes experiments and modeling of thermal and chemical non-equilibrium systems in hypersonic shear layers. In hypersonic flight conditions, gas molecules are in a state of non-thermochemical equilibrium. This research will study interactions of non-equilibrium gas molecules with turbulence.

Accomplishments

Nitric oxide (NO) planar laser-induced fluorescence (PLIF) imaging measurements were performed in a range of flowfields. We used NO PLIF measurements for simultaneous flow-tagging velocimetry and vibrational thermometry in an underexpanded jet. For these measurements, a line of NO was introduced into the flowfield by laser photodissociation of NO2 that was seeded into the flow. Velocities were determined by probing the displacement of the photolytically produced NO using time-delayed NO PLIF imaging. The results were compared to kinetics models and CFD simulations. Efforts to extend this technique to two-component velocity measurements are under way.

A project objective is to achieve NO PLIF measurements that resolve temperature fluctuations of +/– 10 K for mean temperatures of 300 K, necessitating a measurement uncertainty of < 3%. This level of accuracy is challenging to achieve. The effects of detector noise, laser sheet inhomogeneity, and laser attenuation on the temperature measurements were simulated. Results showed that corrections for laser sheet inhomogeneities must be very accurate, and noise can be reduced by judicious smoothing of the temperature images. Temperature uncertainties on the order of 1% were demonstrated by probing the J = 3.5 and 16.5 NO rotational lines in a 300 K chamber, although variations in mean temperatures were +/– 5K due to variations in optical throughput of windows and imaging optics. The addition of flat-field corrections is expected to reduce these variations.

Lastly, rotational temperatures were determined with 1% uncertainty using measurements of N_2(C-B) emission spectra in an RF plasma. The plasma provides a calibration for the NO PLIF measurements.

Significance

Recent accomplishments at Texas A&M represent progress in the application of laser diagnostics to study the coupling between velocity and temperature fluctuations in high-speed turbulent non-reacting flows. Simultaneous flow-tagging velocimetry and T_{vib} measurements may be applied to any flowfield in which NO_2 seeding and NO PLIF imaging are feasible. The use of CARS temperature measurements may be useful for probing energy exchange kinetics between different molecular species downstream of the plasma discharge. Student work at Sandia provided detailed measurements of turbulence scales in jet flows, which will be important for developing accurate simulations of non-reacting jets and jet flames.

Precise Distributed Control and State/Parameter Estimation for Multibody Satellites and Satellite Formations

James Fisher
Texas A&M University

Jeff Spooner (Org. 5338)
Sandia Principal Investigator

Project Purpose

The purpose of this project with Texas A&M University was to investigate approaches to improve closed-loop pointing system performance for Sandia payloads in space applications. In particular this project sought to investigate techniques to help stabilize the line-of-sight of optical sensors to mitigate clutter noise on overhead non-imaging infrared (ONIR) applications when viewing objects with high gradient backgrounds. Typically, when increasing the controller bandwidth to improve closed-loop performance, one runs the risk of decreasing the

stability margins of the system. This then puts the system at risk when system uncertainties encountered (e.g., parameter uncertainties) are outside the range considered in the original design.

Accomplishments

Traditionally, robust control is analyzed by running simulations of various initial conditions and parameter variations, or equivalently, by looking at the frequency domain response for the parameter variations. Given enough mesh points in the parameter variations, this approach is able to provide the designer a good feel for the robustness of a particular closed-loop design.

Within this study, polynomial representations were considered that are able to encompass the system uncertainty. This leads to increased dimensionality of the system states under investigation; however, this dimensionality increase is typically less significant than the parameter mesh requirements of the traditional parameter variational approach. Once the polynomials have transformed the stochastic system uncertainty into a deterministic system, traditional stability analysis and control theory may be used in the design of the feedback algorithms.

Significance

Our work provides a general alternative framework for the design and analysis of closed-loop feedback algorithms when used on systems with parameter (or other) uncertainty. In particular, high-value assets, such as satellite payloads, may benefit from the design of control laws that are robust to particular types of system uncertainties, thereby helping to ensure trouble-free operation throughout its operational lifespan.

Atmospheric Aerosols

Crystal Reed
Texas A&M University

Bernie Zak (Org. 6338)
Sandia Principal Investigator

Project Purpose

The purpose of this project with Texas A&M University is to develop the ambient aerosol chamber for evolution studies (AACES), in order to better understand ambient effects on aerosol transformation. Aerosol chambers have been used in previous laboratory experiments to investigate the coating of gas-phase species on existing aerosols and/or the evolution of aerosols with time. However, previous laboratory results may not have been completely representative of the ambient environment for a variety of reasons. The AACES is designed to avoid the major problems encountered with the use of aerosol chambers in the past.

Accomplishments

We completed a successful field campaign utilizing AACES near Woodland Park, CO, in collaboration with UCAR (University Corporation for Atmospheric Research). AACES is a roughly cubical chamber constructed of a rigid acrylic outer shell, which transmits UV radiation. Teflon lines the inside of the chamber on all sides and the top, while expanded Teflon is used on the bottom of the chamber. The fibrous structure of the latter acts as a barrier to particulates, while allowing gas molecules to move virtually unimpeded from one side of the chamber to the other, creating an initial environment inside the chamber that is free of particles and that continuously reflects the ambient air. We injected monodisperse ammonium sulfate particles into the chamber and monitored the ambient growth process, by determining the peak diameter of the number concentration at any given time and then passing that sample through a humidified differential mobility analyzer to determine associated fractional organic contribution. We are analyzing data collected using the humidified tandem differential mobility analyzer system, to determine the extent of secondary organic aerosol production within a terpene forest. Data will also be compared to that collected by other groups on site in an effort to better understand the processes observed.

Significance

Through the use of the AACES, chemistry models will be better equipped to predict the behavior of the atmospheric aerosols associated with energy production (power plants, refineries, etc.) as well as to better model processes such as the formation of secondary organic aerosols. This will improve the assessment of the environmental impact of such facilities, and eventually, will enable that impact to be minimized.

Spatial Optimization for Regional Storm Water Infrastructure: Balancing Water Quality, Supply Augmentation and Ecosystem Function

Ari Posner
University of Arizona

Vince Tidwell (Org. 6313)
Sandia Principal Investigator

Project Purpose

Through a partnership between Sandia, the University of Arizona, the NSF Science and Technology Center for the Sustainability of Semi-Arid Hydrology and Riparian Areas (SAHRA) and the Pima County Flood Control District, we will develop and demonstrate

a holistic approach and framework for objectively determining the most cost-effective placement and design for storm water infrastructure. This model will be designed to assist water managers in exploring different storm water management options based on discrete watershed characteristics and to be used as both a decision and educational tool.

Accomplishments

Mathematical relationships and the computer models used to simulate storm water channel processes and water quality were identified. The history, development, and governing physics of each program were investigated. Testing of each model was performed for purposes of familiarization and to investigate the capabilities and limitations of each.

Along with data collected by the project team, additional data were collected from both the United States Geological Survey (USGS) and local flood control agencies. The processing of this data has begun, as has the hydraulic modeling of a small section of an arroyo of interest. This arroyo was identified by the team to be of primary interest, and will act as a beta test to determine the data transformations required for the integration of each of the model framework components.

Significance

Storm water facilities are an important infrastructure providing critical flood protection and water quality control. Urban growth coupled with increasing awareness of the severity of nonpoint-source pollution has led communities to enact numerous storm water regulations. Regulations are costly in terms of capital expenditures, power and other resource consumption, and environmental impact. Current design tools fail to take an integrated view of the broad systems impacted and impacting storm water control. Improved tools will provide an expanded basis for storm water planning and design.

Solar Hydrogen Generation with Porous Semiconductor Electrodes

Coleman Kronawitter
University of California, Berkeley

Bonnie Antoun (Org. 8246)
Sandia Principal Investigator

Project Purpose

In this project with the University of California, Berkeley, we are studying solar hydrogen generation as the production of hydrogen fuel using solar-illuminated semiconductor photocatalysts in an electrolytic solution as an attractive renewable energy technology. The research involves the development of film semiconductor photocatalysts with appropriate electronic, optical, and morphological properties to maximize solar absorption as well as catalyze the solar-driven electrochemical production of hydrogen.

Accomplishments

We constructed a gas collection system and calibrated it for the measurement of evolved gas concentrations from photocatalytic reactions. To date, sixteen distinct semiconductor films have been fabricated with some characterization, including zinc sulfide doped with copper, titanium dioxide doped with nitrogen, and an oxynitride blend of gallium nitride and zinc oxide, which have been synthesized under various conditions.

Significance

This research benefits DOE's Science strategic goal by encouraging and developing future world-class scientists that can contribute to advancing scientific knowledge. This research also has great relevance and potential benefit to the DOE's Energy strategic goal. This project will assist development of a technology capable of providing a diverse supply of reliable, affordable and environmentally sound energy.

Mobile Agent Systems for Distributed Embedded System Reasoning and Complex Warfare Simulation

Stephen Nestinger
University at California, Davis

Janson Wu (Org. 8244)
Sandia Principal Investigator

Project Purpose

The purpose of this project was to understand and develop mobile software agents that could be updated in deployed robots/sensors in order to tackle and overcome obstacles and situations that could not be anticipated. This would greatly simplify programming and control required on distributed nodes deployed in the field. This work represents a collaboration with the University of California, Davis.

Accomplishments

Initial stages of the project were successfully completed. We accomplished feasibility testing of the system using a Khepera III K-team mobile robot and two knowledge bases. An empty task agent was able to successfully traverse from the mobile robot to a task knowledge base autonomously and acquire a new task. The task agent then migrated back to the robot and acquired control by communicating with the onboard stationary control agent via FIPA (foundation for intelligent agents)

agent communication language protocols. The task agent then sent behavior provisions to the control agent which spawned a new behavior agent. The behavior agent self-migrated to a behavior knowledge base and acquired the required low-level reactive behaviors for the given task. The behavior agent combined multiple C functions into one agent, each function representing a separate behavior. The behavior agent then migrated back to the robot and informed the control agent of the available behaviors. The control agent then continuously called each behavior function formulating a low level reactive system. If desired, the task agent can subsume the low level reactive system and take full control of the robot.

Significance

Use of these mobile agents could be employed in distributed sensor and response nodes to detect and combat terrorist attacks on critical assets within the United States. It would provide flexible and responsive platforms in the field which could be updated as situations and scenarios change. This embedded reasoning technique provides a step forward toward efficiently deploying and maintaining collaborative in situ processing and fusing of sensor data and management.

Refereed Publications

S.S. Nestinger, B. Cheng, and H.H. Cheng, "A Mobile Agent-based Framework for Flexible Automation Systems," to be published in *IEEE Transactions on Mechatronics*

S.S. Nestinger and H.H. Cheng, "Mobile Agent Framework for Distributed Vision Sensor Fusion," to be published in *IEEE Transactions on Robotics*

Cross-layer Design for Secure Communications in MANETs

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University of California, Davis

Cherita Corbett (Org. 8965)
Sandia Principal Investigator

Project Purpose

In this project with the University of California, Davis, we seek to develop cross-layer techniques to tackle problems related to robustness, reliability, and integrity of ad-hoc networks. A cross-layer solution has the advantage of obtaining more information in decisions made in each layer. We will scrutinize the traditional communication model (internet protocol [IP] based); we will also look into new communication models, based on the concept of social networks, to understand how it could alleviate some of the drawbacks in the current communication model.

Accomplishments

We researched the many attack schemes possible in ad-hoc networks. From the literature research, we observed several trends. First, many of the research works have assumed the use of cryptography whenever identification is required. The use of cryptography has its drawbacks, however. Besides the additional CPU commitment, cryptography does not inherently evaluate the content of the message. That is, messages are sent irrespective of the intention of the sender, as long as the sender has been properly authenticated. Hence, the communication model lacks an inherent method to perform more granulated control over messages. Along this vector, we have also learned that the single-layer approach has its limitations. The separation of knowledge between the layers implies that individual layers might make decisions that exacerbates the performance or compromises the security of a different layer. Thus, cross-layer solutions can complement each layer with additional information to make better decisions. With these observations, we realized that social networking has features that can readily resolve these two problems. Works such as Davis Social Link are looking into a new communication paradigm that builds trust into the network, and interacts with both the underlying routing layer and application layer to correctly choose the correct peer to communicate with. With this, we are currently investigating the development of a collaborative network that utilizes social networking to defend against attacks that aim at false advertisement while following protocol (e.g., black hole, jellyfish attack).

Significance

Contributions of this work can be applied to secure wireless communication and information assurance, which are important to Sandia and the national security.

Fourier Analysis and Synthesis Tomography

Dan Feldkhun
University of Colorado at Boulder

Michael Sinclair (Org. 1824)
Sandia Principal Investigator

Project Purpose

Fourier analysis and synthesis tomography (FAST) is a full-field "synthetic aperture" microscopy technique that does not require a lens to form an image, but provides full-field imaging with millimeters of depth of field, inches of working distance, and submicron resolution. It can achieve KHz imaging rates

and can detect object motion with very high spatial (nm) and temporal (ns) resolution, by tracking the phase of its Fourier components. These capabilities are important for biological applications, such as real-time imaging of signals propagating through neurons and rapid screening of cellular and DNA microarrays, as well as for full-field imaging and motion characterization of microstructures such as microelectromechanical systems (MEMS).

Accomplishments

By making improvements to the optical path of the proof-of-concept (PC-FAST) system, automating it using Labview, and implementing the tomographic filtered backprojection algorithm, our collaborators at the University of Colorado at Boulder were able to synthesize two-dimensional images of an Air Force resolution target and a zoneplate, which were fabricated by ablating chrome on glass using a femtosecond laser. We demonstrated several orders of magnitude improvement over the depth-of-field of a conventional microscope objective with a comparable numerical aperture, and presented these results at the Optical Society of America's (OSA's) biomedical optics conference. However, the two-dimensional reconstructions appeared noisy and of low contrast. We have since made a number of changes to the algorithm and the dynamic range and synchronization of the electronics to improve reconstruction fidelity.

Significance

FAST is a general-purpose image synthesis technique that, unlike lens-based approaches, can maintain very large depth of field and working distance at submicron resolution and can be used to detect nanometer-scale motions. As a result FAST offers benefits to a number of biological science applications such as imaging and tracking of neuron signals, as well as defense and environmental science applications, such as characterization of MEMS actuators and sensors used to detect chemical and biological agents.

The University of Colorado at Boulder has recently been awarded a grant by the National Aeronautics and Space Administration (NASA) to develop a proof-of-concept imaging platform for a future autonomous planetary rover, combining a very large working-distance microscope based on the FAST technology with a high-speed active illumination 3D imaging system that can be used for evaluating science targets and as a real-time terrain navigation aid.

Modeling and Design of Microstructures with Tailored Adhesive Properties

Kevin Sylves
University of Colorado at Boulder

Dave Reedy, Jr. (Org. 1526)
Sandia Principal Investigator

Project Purpose

Our goal is to apply design optimization techniques to structures in adhesive contact where the dominant adhesive mechanism is the van der Waals force. For example, the objective could be matching a force-displacement relationship for an optimization variable of the interface element energy of adhesion. This work was conducted at the Center for Aerospace Structures at the University of Colorado at Boulder.

Accomplishments

Interface finite elements were developed for domains discretized by beam elements, quadrilateral elements or triangular shell elements. The finite element results for problems that include adhesion were compared to analytical solutions. These adhesion problems were then used in optimization calculations, where the objective was matching a force-displacement relationship, and the optimization variables were the interface element energy of adhesion or the width of beam elements in the structure.

Significance

This work relates to ongoing research in microsurface adhesion at Sandia. Applications include self-assembled materials, objects with highly tailored surface adhesion properties and reduction of detrimental adhesive properties in microsystems.

Refereed Publications

K. Sylves, K. Maute, and M.L. Dunn, "Adhesive Surface Design Using Topology Optimization," to be published in *Structural and Multidisciplinary Optimization*

Capture and Utilization of Context in Language Comprehension and Memory

Laura Matzen
University of Illinois at Urbana-Champaign

Travis Bauer (Org. 5635)
Sandia Principal Investigator

Project Purpose

The purpose of this project with the University of Illinois at Urbana-Champaign is to study the human use of context-based cues in language comprehension and memory in order to better understand the structure and organization of human memory

to ultimately improve our ability to process unstructured text.

Accomplishments

We ran two studies to study the susceptibility of young adults to specific types of errors. Second, this study was extended to older adults. Third, we examined factors that may contribute to both true and false memory for surface and semantic information. Fourth, we studied the effects of time. Last, we conducted event-related potential experiments to understand the process of reminding.

Significance

These results improve the general understanding of the S&T community regarding how human memory is organized. They suggest approaches we can take to build technology that mimics human memory. Accomplishing this could improve our ability to deal with large volumes of information and develop modeling and simulation capabilities that mimic human errors for the purpose of simulating environments where surety is critical.

Nanotransport and Control of Molecules Through Molecular Gates

Adam Sawyer
University of Illinois at Urbana-Champaign

Ken Patel (Org. 8621)
Sandia Principal Investigator

Project Purpose

The purpose of the project with the University of Illinois at Urbana-Champaign is to develop sophisticated tools capable of manipulating molecules at their own length scale, thereby enabling new methods for chemical synthesis and detection. Although nanoscale devices have been developed to perform individual tasks, little work has been done on developing a truly scalable platform: a system that combines multiple components for sequential processing, as well as simultaneously processing and identifying the millions of potential species that may be present in a biological sample.

Accomplishments

The research has focused efforts on achieving two major milestones in the development of molecular gate system:

- Investigate new materials for device fabrication to reduce thermal stresses in layers and increase electrical isolation
- Develop a molecular gate–based platform for the polymerase chain reaction (PCR) that includes multiple inlet and outlet microchannels, a central reaction chamber, and an on-chip microheater

Integrating thin metal layers into poly(methyl methacrylate) (PMMA) devices proved challenging due to the large thermal stress cracks and poor electrical isolation produced from the required processing temperatures (200 °C) and mismatch in coefficient of thermal expansion. To address these problems, we developed a new fabrication process, using SU-8, a photodefinable epoxy, for the primary device layers. Since SU-8 can be patterned and crosslinked at only 90 °C, the overall thermal stress in the layers can be significantly reduced. Using a hybrid substrate, thermal stresses could be further reduced, leading to crack-free layers. Electrical measurements indicate leakage currents two orders of magnitude lower for SU-8 layers when compared to PMMA.

Significance

Development of molecular gates as a scalable architecture for controlling molecules and nanotransport is a vital part of DOE's mission to advance scientific understanding of nanoscale phenomena. Tools to help understand nanoscale transport will ultimately lead to the development of new diagnostic devices and methods to explore alternatives to environmentally sound energy sources.

Multi-Mode Energy Scavenging from the Environment

Tzeno Galchev
University of Michigan

Chris Apblett (Org. 1815)
Sandia Principal Investigator

Project Purpose

The purpose of this project is to develop a micro power generator, which can efficiently scavenge energy from low-frequency ambient vibrations. We are exploring a new technique known as frequency up-conversion, which can increase the mechanical efficiency of this generator at low-frequencies. The basic operation is that energy is coupled from the environment to a low-frequency sensitive resonator, which then passes a portion of this energy to a second resonant element that is used for conversion, operating at a higher frequency. This project represents a collaboration with the University of Michigan.

Accomplishments

We have analyzed the frequency up-conversion technique in more detail. Simulations show that using two devices with a specific mass ratio can lead to a 36% improvement in energy density when using frequency up-

conversion over other approaches. An electromagnetic microgenerator which occupies a volume of 5.7 mm^3 has been designed. This generator is optimized to work at 110 Hz, and produce 32 µW from an input vibration of 1 g. We have overcome fabrication challenges associated with the generator's geometry and necessary critical feature size. We have developed a process technology that can effectively create the 9.13-milligram suspended mass with an integrated coil for electromagnetic transduction. Testing of the device is under way.

Significance

If successful, this method of harvesting mechanical power can produce efficiencies above the simple springboard resonator type harvesters that have currently been demonstrated.

Diffusion-based Sensing of Membrane Proteins in Solid Support Platforms

Jason Cox
University of New Mexico

Susan Brozik (Org. 1714)
Sandia Principal Investigator

Project Purpose

In hopes of unlocking some of the fundamental biophysical questions in membrane-bound protein systems, our goal was to develop new ways to study representative proteins in synthetic platforms that aid in probing these molecules using optical techniques. In terms of single-molecule fluorescence measurements, two challenges constantly arise, (1) the labeling of important biological molecules, and (2) sample preparation. In collaboration with the University of New Mexico, we wanted to demonstrate a general method for synthesizing a variety of fluorescent conjugates of 5-hydroxytrypamine (serotonin) and present a single-molecule fluorescence imaging study describing the binding of this new serotonin agonist to a ligand-gated ion channel.

Accomplishments

In this project, our group has been working toward the characterization of the ligand-gated, ion channel, human serotonin type 3 receptor, (5HT3R). Specifically, we were interested in answering some of the fundamental biophysical questions that pertain to this protein in native and synthetic environments; including evaluation of specific parameters such as the binding coefficients and allosteric motions that accompany ligand binding and how these events relate to channel opening. In pursuit of these questions, we have successfully incorporated 5HT3R into self-assembled, supported, lipid bilayers on planar substrates and nanoporous silica beads. This was a huge achievement, because these synthetic platforms have greatly simplified the characterization of membrane proteins and have led to the following accomplishments:

- Development of electrochemical and optical assays for assessment of function for the ligand-gated ion channel, (5HT3R)
- Measurement of membrane fluidity using fluorescence correlation spectroscopy

Additionally, we were interested in studying the binding events that lead to the ion channel opening and closing. To this end, we have developed a general synthetic scheme that allows us to conjugate virtually any amine reactive fluorescent dye molecule to the receptor agonist, serotonin.

- Developed a general strategy for protein labeling and synthesized two, novel fluorescent agonists to 5HT3R
- Designed a sample preparation that allows for the use of fluorescence resonance energy transfer (FRET) between ligand and receptor, providing a selective binding assay

Significance

Membrane-bound proteins have been identified as a major target for therapeutics and for their potential in biosensing technologies. Implementing these complex biological structures into controlled environments presents an important challenge for the realization of future innovations. Our work developing supported bilayers on nanoporous silica microbeads as stable environments for proteins represents new discoveries and advances in nanomaterials which can now be applied toward basic protein research or the development of sensitive, integrated devices that can be used to detect and identify biological agents.

Nanostructured Electrocatalyst for Fuel Cells: Silica Templated Synthesis of Pt/C Composites

Elize Switzer
University of New Mexico

Cy Fujimoto (Org. 6338)
Sandia Principal Investigator

Project Purpose

The essential balance of kinetic and transport properties of methanol oxidation electrocatalysts are due, in part, to the hierarchical structure that combines distinct structural considerations across length scales. The result of this type of structure is a relatively low surface area for catalysis, which results in inefficient mass transport within the fuel cell catalytic layer. This work with the University of New Mexico will assist in understanding these properties

as well as in pursuing synthesis of enhanced materials through investigation of novel bimetallic Pt-Ru nanowire networks.

Accomplishments

We explored the synthesis processes and electrochemical activity of nanostructured Pt-Ru nanowire and particle networks. Once the ability to alter and fine-tune the Pt-Ru microstructure exists, fundamental studies of the local structures can be undertaken. By controlling the morphology of the Pt-Ru catalyst on the nanoscale, the effects of the local structure on electrochemical activity can be studied and a new class of catalysts developed.

We employed an innovative aerosol-based synthesis approach that involves using silica to template Pt and Ru precursors, followed by silica removal for structured electrocatalysts. The structuring of the electrocatalyst on the nanoscale creates advantages in the local mass transfer properties. These improvements result in an improved balance of kinetic and transport properties of the electrocatalysts, due, in part, to the hierarchical structure which combines distinct structural considerations across length scales. The catalyst precursor solution consists of colloidal silica particles with an average diameter of 20 nm, and metallic-amine platinum and ruthenium complexes. In this method of synthesis, all phases are in intimate contact during synthesis which promotes the production of a homogeneous material with a higher degree of alloying.

Significance

Work in this area is of interest to the DOE Energy Efficiency and Renewable Energy (EERE) division, which is currently seeking cheaper and active electrocatalysts. This work has shown promise with non-noble metal activity, which in an alkaline environment, rivals platinum.

Refereed Publications

E. Switzer, M.C. Hibbs, and P. Atanassov, "Alkaline Fuel Cell Eletrocatalyst," to be published in the *Journal of Electrochemical Society*

Advanced Materials for Water Treatment Membranes: Enhanced Rejection Performance and Surface Properties

Elizabeth van Wagner
University of Texas at Austin

Susan Altman (Org. 6338)
Sandia Principal Investigator

Project Purpose

This project aims to leverage the biofouling testing capabilities of Sandia and the capabilities in membranes, transport measurements, and water purification technologies at the University of Texas at Austin. The purpose of this work is to create new polymer membranes that have high flux for pure water, but are able to reject salt and have good fouling resistance. We plan to fabricate dense layers of functionalized poly(phenylene) and poly(aniline) on porous supports and test these membrane concepts for their performance in water purification bench-scale experiments.

Accomplishments

We have conducted a baseline characterization of commercial (unmodified) reverse osmosis membranes. We found that variables such as feed pH and the use of continuous feed filtration proved to have significant impact on the measured performance (i.e., water flux and salt rejection) of the commercial membranes. In addition, we discovered that system cleaning protocols and membrane storage, handling, and pretreatment were also important factors to control. Currently, a manuscript detailing the results of these studies is in preparation, with plans to submit it to the *Journal of Membrane Science.*

In addition, we have developed a hybrid method of dip coating and spin coating to modify the surfaces of commercial membranes. The hybrid method involves only contacting the top surface of the membrane with the treatment solution, similar to the contact provided during spin coating, but without rotating the membrane to spread the solution, which was found to lead to inconsistent surface coverage. We are conducting modifications on a higher-flux nanofiltration (NF) membrane. This membrane has the same surface chemistry as the reverse-osmosis (RO) membranes, and therefore has the same reactive surface groups available, but has a looser structure, indicated by higher water flux and lower salt rejection than the RO membrane. Using higher molecular weight poly(ethylene glycol) diglycidyl ethers (PEG diepoxides) grafted to the NF membrane surface, we were able to increase the salt rejection to levels comparable to the commercial RO membrane. Crossflow fouling studies using charged surfactants indicated these PEG-modified NF membranes have better fouling resistance (i.e., less flux loss upon addition of foulant to the feed), as well as flux recovery upon cleaning as compared to unmodified control RO membranes with similar initial water flux and salt rejection properties.

Significance

Membranes are the technology of choice for water purification. Reverse osmosis processes produce high-purity water from saline water, but polyamide membranes, the state of the art, do not have good fouling resistance and their fundamental properties are poorly understood in terms of the mechanisms of salt rejection.

This project supports technology and materials testing capability development in the area of water purification, which is of strategic interest to Sandia and may provide future opportunities for programmatic work.

Dynamics of Propagating Shock Waves and Phase Fronts

Johnathan Niemczura
University of Texas at Austin

John Pott (Org. 1524)
Sandia Principal Investigator

Project Purpose

This research project with the University of Texas at Austin examines the dynamics associated with the generation and propagation of shock waves and phase fronts in solids. Such phase transformations and shocks are developed in many high-energy impact and explosion problems; understanding the physics of these phenomena in a wide range of materials permits their use in structures designed to mitigate the effects of blast or impact events. This research involves a combination of experimental observations, analytical modeling, and numerical simulations of models.

Accomplishments

- Developed an analytical model of tensile impact of rubber and ran numerical simulations that quantitatively match the experiments
- Carried out tensile impact experiments on NiTi using digital image correlation and captured the strain field over the entire specimen during the propagation of the phase front, allowing the calculation of the kinetic relation

Significance

This research aims to develop the mechanics of shock propagation for materials exhibiting phase transformation. While this research is of great interest for the enduring stockpile, more importantly, it may also enable the future insertion of tailored materials for shock and vibration mitigation.

Rapid Manufacturing Innovations for Monitoring Systems

Contract Research
University of Texas at El Paso

Jeremy Palmer (Org. 2617)
Sandia Principal Investigator

Project Purpose

The purpose of the project is to realize dramatic near-term benefits through focused application of rapid manufacturing (RM) technology in fabrication of components for advanced monitoring systems. A primary research objective is to reduce engineering development cycle time for electro-optomechanical components by investigating, (1) novel ultrasonic consolidation of aluminum and electron beam melting (EBM) of titanium to generate complex part geometries; (2) high aspect ratio three-dimensional direct write (DW) interconnect for thick multilayer printed wiring boards (PWBs) and, (3) plated RM composites with superior outgassing performance.

Accomplishments

Through our collaboration with the University of Texas at El Paso (UTEP), we performed statistical analyses to determine the effects of build orientation on ultimate tensile strength and Young's modulus for stereolithography (SL) manufactured parts — this research is required to determine the ability of existing additive layered manufacturing systems to produce rapidly manufactured end-use parts (instead of simply providing prototypes). Specifically, this research effort is, (1) developing statistical methodologies that can be used to characterize dimensional and mechanical property variations of parts produced in varying orientations using additive layered manufacturing technologies; (2) applying these statistical methodologies to test samples built using SL; and (3) exploring possible strategies for removing the effects of part build orientation on dimensional accuracy and mechanical strength. Results have been summarized in a journal paper submitted to the *International Journal of Advanced Manufacturing Technology.*

We sought to advance the integrated manufacturing system that combines an SL-additive layered manufacturing machine with a DW fluid-dispensing system for the automated manufacturing of three-dimensional electronic devices. This work has led to a joint UTEP/Sandia patent application entitled, "Methods and Systems for Integrating Fluid Dispensing Technology with Stereolithography."

We also explored the possibilities of using the Arcam A2 electron beam melting (EBM) additive-layered manufacturing system for producing Ti-6Al-4V satellite components. Current research is exploring the ability to start and stop the EBM process so that integrated Ti-6Al-4V assemblies can be manufactured directly on the EBM system. If successful, the EBM system will be able to effectively provide complicated satellite components as a single component that previously required accurate assembly of multiple components.

Significance

The key accomplishments have the following impacts. First, assemblies of metallic components can be fabricated as monolithic parts to save mass and volume. Second, and perhaps most far-reaching, is that cost-effective multifunctional modules can be created that include three-dimensional electronic, structural, and thermal elements. These may dramatically reduce mass and volume while improving performance in flight environments.

Active Control of Periodic Disturbances

Scott Pigg
University of Utah

Gene Hertel, Jr. (Org. 1516)
Sandia Principal Investigator

Project Purpose

The objective of this research with the University of Utah is to investigate algorithms for the rejection of unknown disturbances, with a particular interest in active noise and vibration control applications (ANC, AVC, or ANVC). Disturbances are assumed to be the sum of periodic signals with time-varying magnitudes, frequencies, and phases. Feedback control algorithms, where no reference sensor is available to provide a preview of the disturbance, are of primary interest. These problems are more difficult to solve and less well understood. The algorithms are also able to handle systems with unknown and possibly time-varying dynamics.

Accomplishments

We developed new algorithms for rejection of periodic disturbances. The focus on known periodic disturbances makes this research relevant to many applications involving rotating equipment. Adaptive feedback control has been considered, in which knowledge of the disturbance frequency and plant dynamics allows for perfect cancellation of periodic disturbances. Algorithms that identify and adapt to variations in disturbance or plant parameters have been considered.

Since many applications involve unknown and time-varying dynamics due to variations in environmental factors, we developed methods for identifying plant parameters online. We have implemented and investigated several such methods on an active noise control test bed. One technique involves the use of gradient or conventional least-squares identifiers to update an estimate of the plant, allowing estimation of the parameters to occur continuously and without the need for any added excitation. Averaging theory was used to gain insight into stability properties of algorithm and has shown that parameter convergence obeys certain well-defined constraints. ANC experiments were used to verify results of the analysis, and we have observed the significant attenuation of sinusoidal disturbances.

Many sources of periodic disturbances experience frequency drift. This involves the slow movement of the frequency away from the initial steady-state value. As such, techniques that adapt to changes in both the system dynamics as well as the disturbance frequency have been considered. Due to the interaction of the various components, adding frequency estimation leads to additional complication of the dynamic response. In order to derive methods that posses desired robustness properties and perform well with respect to changing dynamics. We have exploited the various stability characteristics of batch algorithms, where parameters are extracted by processing batches of consecutive samples, and continuous algorithms, which update parameter estimates with each new sample. The significant attenuation of sinusoidal disturbances has been observed in ANC experiments.

Significance

In active noise and vibration control applications, the number of parameters needed to describe the system is much smaller than the number required to describe the transfer function in ANC systems. Of interest, here, are feedback structures which require no reference sensor to give a preview of the disturbance. Using batches of consecutive disturbance cancellation error measurements, robust structures can be derived, and changes in the system can be tracked in real time. By combining approaches, robust structures able to quickly respond to time variation are possible. Similar algorithms can be used for active noise control and active vibration control.

Richtmyer-Meshkov Instability of a Membraneless Gas Interface

Bradley Motl
University of Wisconsin-Madison

Randall Summers (Org. 1431)
Sandia Principal Investigator

Project Purpose

The purpose of this project was to experimentally explore the Richtmyer-Meshkov (RM) instability as a function of Atwood number and shock strength in collaboration with the University of Wisconsin-Madison. This stability is of interest to researchers in the fields of inertial confinement fusion, astrophysics, and hypersonics where the turbulent mixing may enhance or degrade a desired or observed result.

Accomplishments

We conducted an experimental parameter study of the RM instability for a sinusoidal, membraneless interface in a vertical shock tube for a range of Atwood numbers ($0.29 < A < 0.95$) and shock strengths, $1.1 < M < 3$. The RM instability occurs when a perturbed interface between two fluids of differing densities is impulsively accelerated, and ultimately leads to the turbulent mixing of the two fluids. We used planar imaging techniques to diagnose a nearly single-mode, two-dimensional gas interface. Amplitude growth rates in the linear and nonlinear regimes were measured and compared to several analytic models and Lawrence Livermore National Laboratory's hydrodynamics code, Raptor. We obtained results for eight scenarios, which include three interface gas pairs. We characterized the initial condition for each gas pair, and results indicated that the interface is predominantly single-mode and two-dimensional for a specified region of interest within the shock tube. Shocked interface visualization results reveal the presence of qualitatively different features and growth rates for each Mach/Atwood number scenario. Experimental data, presented in a non-dimensional format, compare well with single-mode results from Raptor. The non-dimensional scaling collapses the experimental data to a single line from early to moderate non-dimensional times. The experimental and Raptor amplitude growth rate data show best agreement with a model proposed by Mikaelian across the studied parameter space.

Significance

The experimental data obtained can be used as a test matrix to evaluate various hydrodynamic computer codes and analytical models. This study is the first to investigate the Richtmyer-Meshkov instability for a He/SF_6 interface, which has an Atwood number approaching unity. These results will be of great interest to the inertial confinement fusion community, which designs fusion fuel pellets that may have an Atwood number approaching one. This study is also the first to conduct membraneless experiments for a Mach number approximately equal to, and greater than, M=2.

Refereed Publications

B.J. Motl, J.H. Niederhaus, D. Ranjan, J.G. Oakley, M.H. Anderson, and R. Bonazza, "Experimental Study for ICF-related Richtmyer-Meshkov Instabilities," *Fusion Science and Technology*, vol. 52, pp. 1079-1083, November 2007

Using Reconfigurable Functional Units in Conventional Microprocessors

Kyle Rupnow
University of Wisconsin-Madison

Arun Rodrigues (Org. 1422)
Sandia Principal Investigator

Project Purpose

This project with the University of Wisconsin–Madison examines the limiting factors in Sandia supercomputing application performance. Our work, thus far, demonstrates that integer computations constitute a surprisingly large percentage of Sandia floating point applications. These integer computations primarily generate memory addresses, and are thus an important part of overall application performance. Dataflow graphs formed by these instructions are large and complex. Our work will examine the extent to which the performance of these graphs affects memory system and overall performance of the applications. We also propose several techniques to accelerate these dataflow graphs.

Accomplishments

Initial work demonstrated that Sandia applications have significantly more integer instructions than standard performance evaluation corporation floating-point (SPEC-FP) benchmarks, and that these integer instructions primarily calculate memory addresses for complex data structures. Therefore, optimizing an architecture to SPEC-FP may not result in an architecture also optimized to Sandia applications.

We also developed a reconfigurable functional unit (RFU) to accelerate integer computation, with a coarse-grained architecture whose design is based on Sandia application characteristics. We added design features specifically to support large and complex dataflow based on Sandia application needs. Although this technique would work well for an embedded-type processor, it is not as effective when combined with high-performance central processing units (CPUs) normally used in scientific computing. Acceleration was 3% on average, with a maximum acceleration of 12%.

Therefore, we are modifying the focus of this work to incorporate dynamic binary optimization. In addition to existing dynamic optimization techniques, an optimizer will translate sections of application code to the RFU at run-time, making optimizations that were not possible with a compile-time approach. Furthermore, this would permit binary compatibility between augmented and non-augmented architectures. These efforts will have numerous other potential benefits, including easier migration between systems and improved fault tolerance.

Significance

The technical achievements have the potential to influence system design of next-generation supercomputers and lower development effort to efficiently use the heterogeneous resources likely to be available in these systems. Next-generation CPUs, and therefore, supercomputers will be multicore, and these cores will likely be heterogeneous. Dynamic binary optimization can perform complex optimizations not possible at compile time due to library mappings and data dependent behavior. This project targets transparent and binary compatible acceleration of applications.

PRESIDENTIAL EARLY CAREER AWARDS FOR SCIENTISTS AND ENGINEERS

DOE/NNSA Defense Programs (DP) identifies nominees for the Presidential Early Career Awards for Scientists and Engineers (PECASE) from the most meritorious recipients of the DOE/NNSA-DP Early Career Scientist and Engineer Award. Candidates for this award are researchers employed by academic institutions who are in the first five years of their independent research careers. Individuals are nominated by directors of DP laboratories based on the candidate's contribution to the DP mission. Up to six winners are selected annually by the Office of Defense Programs from the nominations provided by the laboratory directors. Up to three of the winners of the DP Early Career Scientist and Engineer Award may also be designated annually by the laboratory directors as DP nominees for the PECASE. The nominating laboratory is responsible for funding the PECASE awardee for the next five years.

The PECASE embodies the high priority placed by the government on maintaining the leadership position of the United States in science by producing outstanding scientists and engineers and nurturing their continued development. The awards identify a cadre of outstanding scientists and engineers who will broadly advance science and the mission. Further, the awards foster innovative and far-reaching developments in science and technology, increase awareness of careers in science and engineering, give recognition to the scientific missions of participating agencies, enhance connections between fundamental research and national goals, and highlight the importance of science and technology for the nation's future.

The award is $250,000, given to the awardees through a $50,000 per year research contract funded through the Laboratory Directed Research and Development (LDRD) Program. This provides the awardee an opportunity to continue research in the area for which he/she was nominated and for Sandia to benefit from the results of the developments.

Discontinuous Galerkin Methods for Generalized Continuum Models for Inelasticity

Krishna Garikipati
University of Michigan

Jay Foulk (Org. 8246)
Sandia Principal Investigator

Project Purpose

This project involves the development of a class of new finite element methods, based on the discontinuous Galerkin (DG) method, which makes possible the numerical solution of complex, strain gradient continuum models with standard, C0 finite elements. These strain gradient continuum models of plasticity and damage typically involve high-order (usually fourth-order) spatial derivatives, which prevent their numerical solution via standard, C0 finite element methods. This project represents a collaboration with PECASE (Presidential Early Career Award for Scientists and Engineers) recipient, Dr. Krishna Garikipati, at the University of Michigan.

Accomplishments

The University of Michigan group is now working on two types of discontinuous Galerkin (DG) formulations for the incompatibility-based strain gradient plasticity model. These are the interior penalty and lifting operator formulations. Preliminary results using the interior penalty DG formulation were presented at the International Union of Theoretical and Applied Mechanics (IUTAM) Symposium on Theoretical, Modelling and Computational Aspects of Inelastic Media, held in Cape Town, South Africa, January 14–18, 2008.

We are currently developing a solution algorithm for the equations in which the plastic flow rule is solved in a staggered fashion with the equilibrium equation. This algorithm works for problems with and without incompatible plastic deformation, and is applicable to the interior penalty and lifting operator formulations.

Significance

The field of plasticity, and particularly computational plasticity is in very early stages of the development of finite element methods for strain gradient continua. Strain gradient continuum models of plasticity and damage provide a means to link length scale effects (which originate at the grain and subgrain scale in metals) to macroscopic models of mechanics.

These methodologies are of particular interest to Sandia. From designing microsystems to modeling component failure in abnormal environments, the numerical methods developed in this effort may provide a means to include the requisite physics and obtain regularized (mesh-independent) solutions.

Refereed Publications

J. Ostien and K. Garikipati, "A Discontinuous Galerkin Method for an Incompatibility-based Strain Gradient Plasticity Theory," in proceedings of the IUTAM Symposium on Theoretical, Modelling and Computational Aspects of Inelastic Media, 2008

Developing Novel Scaffolds for Biological Molecules by Solving the I-QSAR Problem Using the Signature Molecular Descriptor

Don Visco
Tennessee Technological University

Elebeoba May (Org. 1412)
Sandia Principal Investigator

Project Purpose

This project with PECASE recipient, Donald Visco at Tennessee Technological University, has two purposes. First, the primary purpose is to evaluate the molecular descriptor, "Signature," for its utility in high-throughput screening (HTS) studies. A vast amount of information exists in public databases (such as PubChem) concerning the activity of molecules against certain protein targets. With Signature, in conjunction with support vector machine (SVM) classifications and powerful clustering/feature selection techniques, information can be mined from the databases to make predictions on the activity of compounds not yet tested against a particular protein target. The second purpose is to continually evaluate Signature for use in inverse-design problems.

Accomplishments

We focused on evaluating Signature for use in HTS. Initially, the idea was to study promiscuous inhibitors, but that was superseded by a general method to classify factor XIa inhibitors from PubChem using Signature and an SVM classification. Our technique was successful on a balanced set and the rest of PubChem (10+ million compounds) was screened against this classifier. Using an internally developed metric that provides a confidence on predicted values, we identified several hundred for further

study. These compounds were docked successfully in the binding pocket of the protein and contain several that have a low similarity with the original bioassay in PubChem. Such compounds represent nonintuitive structures predicted to have activity, which may open up a new class of inhibitors for factor XIa. In addition to this work, inverse design studies using Signature were performed on developing novel corticosteroids which have been predicted to have high receptor binding affinity, high systemic clearance, high plasma protein binding and low oral bioavailability.

Significance

There are very few published works that explore mining of the PubChem database. This work is significant because it provides a successful demonstration (using Signature) of how this can be accomplished, and has been recently accepted for publication in the journal, Molecular Graphics and Modeling. In the next phase of the study, we are exploring dozens of balanced bioassays in PubChem, using this technique in an automated approach.

Signature, whether used in the solution of the inverse design problem or as the means for similarity searching via chemical alignment, provides the potential to generate compounds that possess a desired property or activity. Accordingly, once these techniques mature, they can be used as a means to develop compounds that see application in protecting our national security.

Rheological Properties of Nanocomposites

William King
University of Illinois at Urbana-Champaign

Blake Simmons (Org. 8625)
Sandia Principal Investigator

Project Purpose

The purpose of this project is to understand the rheological properties of polymers and filled polymer composites at the nanoscale. This project is in collaboration with PECASE recipient, Professor William King at the University of Illinois, Urbana-Champaign.

Accomplishments

We are using one of the tools in Professor King's laboratory: a heatable silicon probe tip that is about 10 nm in size. The heated tip can be used like the world's smallest soldering iron, in a technique known as thermal dip pen nanolithography. The tips can write nanometer-scale patterns directly onto a variety of surfaces. In another application, he has used the heated probes to grow carbon nanotubes and to study their growth under different conditions. Because the probes can be heated and cooled more rapidly than traditional furnaces, they can produce nanostructures hundreds of times faster than traditional processing techniques. In another different application, he has used the heated probes to perform measurements of glass transition with 100-nm resolution. This is a major improvement over previous commercially available tools that could achieve resolution near 10 micrometers. The hundredfold resolution improvement makes this technique useful to nanotechnologists who are developing new pharmaceuticals and polymer composites. We have used these tools to analyze the rheological properties of thermoplastic polymers and nanocomposites. This work has resulted in unprecedented new insight into the behavior of constrained polymer films at the nanoscale.

Significance

The thermal processing techniques developed in the King group are useful for a wide variety of micro- and nanomanufacturing applications that are scalable to industrially relevant applications and materials, and will support Sandia's mission in nanotechnology and nuclear weapons. These applications include nanomanufacturing of tissue scaffolds for biotechnology, nanofabrication of ultrahydrophobic water-repellant surfaces, and incorporation of aligned carbon nanotubes into flexible plastic sheets.

Refereed Publications

F.T. Goericke, J. Lee, and W.P. King, "Microcantilever Hotplates with Temperature-compensated Piezoresistive Strain Sensor," *Sensors and Actuators A*, vol. 143, pp. 181-190, May 2008

Aligned Mesoporous Architectures and Devices

Yunfeng Lu
University of California at Los Angeles

Jeff Brinker (Org. 1002)
Sandia Principal Investigator

Project Purpose

During the last decade, mesoporous materials with tunable periodic pores have been synthesized using surfactant liquid crystalline as templates, opening a new avenue for a wide spectrum of applications. However, their applications are somewhat limited by their unfavorable pore orientation. Although a great effort has been devoted to align the pore channels,

fabrication of mesoporous materials with perpendicular pore channels remains challenging. With PECASE recipient, Dr. Yunfeng Lu, at the University of California, Los Angeles, we are exploring the use of the aligned architectures for ionic transport channels. Success of this work may provide new synthesis insight leading to better materials for many energy-related or biological applications.

Accomplishments

Our work has demonstrated that pore channels of mesoporous silica can be aligned using capillary force. This was achieved by contacting a nanocomposited thin film that contains inorganic clusters or oligomeric building blocks and lytropic surfactant liquid crystalline phase with an anodized porous alumina membrane. Wetting of the nanocomposite on the porous membrane creates fluid meniscus, generating capillary force that fills the alumina pore channels with the nanocomposite. During the capillary rise, the mesostructure within the nanocomposite was aligned by shearing force and formed aligned mesoporous channels after further polymerization and surfactant removal. This work leads to the formation of long fibers or fiber bundles with aligned pore channels.

We demonstrated alignment of hexagonal pore channels within porous anodized alumina membranes using capillary forces, as outlined below:

- Optimized the synthesis condition to achieved highly aligned mesostructure
- Synthesized polymer-based fibers with aligned pore channels
- Set up a protocol for neuron signal transmission experiments

Significance

Demonstration and characterization of transport through aligned architectures that simulate ionic channels is key to applications in fuel cells and neuron signal transmission. Success of this work may provide a new synthetic approach to novel architectures, as well as insights that may lead to enhanced materials for many energy-related or biological applications.

Refereed Publications

L. Yang, H. Peng, K. Huang, J.T. Mague, H. Li, and Y. Lu, "Hierarchical Assembly of Organic/ Inorganic Building Molecules With π-π Interactions," *Advanced Functional Materials*, vol. 18 (10), pp. 1526-1535, May 2008

D. Pan, L. An, Z. Sun, W. Hou, Y. Yang, Z. Yang, and Y Lu, "Synthesis of Cu-In-S Ternary Nanocrystals with Tunable Structure and Compositions," *Journal of the American Chemical Society*, vol. 130 (17), pp. 5620-5621, April 2008

Z. Yang, J. Wang, K. Huang, J. Ma, Z. Yang, and Y. Lu, "Functional Mesoporous Polymers from Phenolic Building Oligomers," *Macromolecular Rapid Communications*, vol. 29 (5), pp. 442-446, March 2008

On the Role of Numerical Error in Turbulence Simulations

Christopher Roy
Virginia Technical University

Ryan Bond (Org. 1515)
Sandia Principal Investigator

Project Purpose

Because of the difficulties in isolating numerical and modeling errors in turbulence simulations, new approaches are needed to assess numerical errors. One promising approach, which we are investigating with PECASE recipient, Christopher Roy of Virginia Tech, is the method of nearby problems (MNP) where exact solutions are generated via spline fitting of highly resolved numerical solutions. If nearby problems can be generated in four dimensions (three spatial dimensions plus time), then they can provide a test bed for evaluating the dissipative and dispersive behavior of different numerical schemes on realistic problems. This is especially critical when assessing dissipative numerical schemes, such as second-order upwind schemes which are commonly used for compressible flows containing shock waves.

Accomplishments

We successfully extended the MNP from 1D to multiple dimensions with a general approach that can be extended to 3D and 4D problems in a straightforward manner. Successful implementation of multidimensional MNP will allow for the development of a unique test bed of realistic flow problems for evaluating different numerical discretization schemes used in unsteady turbulence simulations. We then focused on generating realistic, two-dimensional, exact solutions for the heat conduction and Navier-Stokes equations with small source terms, and also include the extension of the spline-fitting procedure to higher dimensions. The 2D applications on which we have focused include 2D heat conduction with a distributed source term and steady, incompressible, viscous flow in a 2D lid-driven cavity. The latter case is challenging due to the two singularities that occur when the moving lid meets the stationary sidewalls. The MNP approach was shown to provide estimates of the discretization error that are comparable to those from Richardson extrapolation, but which require a solution only on a single grid level.

Significance

The method of nearby problems (MNP) provides a test bed of realistic exact solutions for evaluating the behavior of different numerical schemes. This is especially critical

when assessing dissipative numerical schemes, such as second-order upwind schemes commonly used for compressible flows containing shock waves. This application is not limited to computational fluid dynamics, but is applicable to the broader area of computational science and engineering. In addition, MNP has shown promise as a single-grid discretization error estimator. Numerical errors contribute to the overall uncertainty of a simulation prediction, and thus, must be estimated when assessing the predictive capability of any modeling and simulation tool.

Fundamental Studies of Electrokinetic Phenomena in Polymer Microsystems

Brian Kirby
Cornell University

Blake Simmons (Org. 8625)
Sandia Principal Investigator

Project Purpose

The purpose of this project with PECASE recipient, Brian Kirby at Cornell University, is to understand the phenomenon of electrokinetic transport at the nanoscale. The knowledge generated by this project will enable the tailoring of surface chemistries of materials used in next generation micro- and nanofluidic devices, and will enable breakthroughs in applications relevant to homeland security and energy security.

Accomplishments

Among the unique properties of microfluidic devices is the ability to move liquids via electro-osmosis. When the solid-liquid interface acquires a surface charge, an electrical double layer is formed as ions in the electrolyte solution align preferentially based on their charge. When this occurs, an electric field applied parallel to the wall will induce fluid flow.

Modeling and predicting the electrokinetic properties of microfluidic substrates that lead to electro-osmosis is inherently difficult. The surface charges are a function of chemical reactions and adsorption/desorption processes, many of which are not fully understood. Further, the electrical double layer is often nanometers thick, and bulk fluid properties typically do not apply close to the wall, where the highest charge density (and therefore most of the action) resides.

Our work on the electrokinetic properties of microfluidic substrates includes (1) experimental characterization of interface properties, (2) chemical modification of interface properties, and (3) analytical and numerical modeling of double layer phenomena.

We have characterized the electrokinetic properties of hydrophobic microchannel substrates, with specific attention to temperature and solvent properties. Preliminary data show dramatic effects due to solvent addition on Zeonor substrates, with characteristic decay times on the order of seven hours, which we hypothesize is related to the formation of pseudostable nanobubbles at the interface.

Significance

The knowledge generated by this project will enable the realization of next-generation microfluidic systems. These systems will have widespread applications in support of several Sandia missions, including homeland security, nonproliferation, and energy security.

President Harry S. Truman Fellowship in National Security Science and Engineering

University Research, in partnership with Human Resources, established the President Harry S. Truman Fellowship in National Security Science and Engineering Program (Truman Fellowship) in 2004. This program provides an opportunity each year for exceptional scholars to join Sandia National Laboratories (Sandia) in the continuation of Sandia's tradition of excellence. The Fellowship is named for President Harry S. Truman who, in 1949, asked AT&T to accept managerial responsibility of Sandia and challenged us to provide "an exceptional service in the national interest"—a motto that drives us to excel to this day.

The Truman Fellowship seeks to attract the best nationally recognized, new PhD scientists and engineers. It provides the opportunity for recipients to pursue independent research of their own choosing that supports Sandia's mission. The appointees are expected to foster creativity and to stimulate exploration of forefront science and technology and high-risk, potentially high-value R&D. Fellowships are for three years and are funded through the Laboratory Directed Research and Development (LDRD) Program.

Truman Fellowship candidates are expected to have solved a major scientific or engineering problem in their thesis work or have provided a new approach or insight to a major problem, as evidenced by a recognized impact in their field.

In 2008, two additional Fellows were selected. They came to Sandia from the Swiss Federal Institute of Technology and the University of Arizona. They joined four Fellows who had previously competed for the Truman Fellowship.

2008 TRUMAN FELLOWS

Dr. Anatole von Lilienfeld received his PhD at the Swiss Federal Institute of Technology in 2005 and subsequently held postdoctoral appointments at the University of California at Los Angeles and New York University. Anatole's research proposal for the Truman Fellowship, "Multiscale Schemes for the Predictive Description and Virtual Engineering of Materials", brought together the collective skills he acquired toward the development of multiple length-scale computational tools that may be used in the molecular material design. His proposal addresses the quantum mechanics/MD and the extension to density functional theory (DFT) and the unsolved problem of predicting crystal structures. He plans to apply a variational multiscale approach in optimizing material properties at the continuum scale. His vision is to apply these techniques in the development of specialized materials, such as the design of a catalyst that would convert water to hydrogen fuel. Dr. von Lilienfeld's research speciality, theoretical chemistry, is of great interest to many groups at Sandia, particularly in Organization 1400. His expertise and interests will complement and enhance computational material studies being done at Sandia in areas such as high energy density physics, molecular electronics, explosive materials, energy production/storage, bio-hazards, rational material design, etc. He joined Sandia in April 2007.

Dr. Darin Desilets built a whole new technical field, "Cosmic Ray Metrology", the quantification of cosmic ray flux attenuation at the Earth's surface and its application to understand such things as: water balances in soils, global climate change, and earthquake dynamics. Dr. Desilets also demonstrated a national security application - specifically, how the approach might be used to rapidly track the movement of large numbers of people in urban areas. His ability to combine cosmic ray physics, statistics, and hydrology using multiple sensing platforms to address a broad variety of problems suggests that he can contribute to a number of Sandia mission areas – particularly in Organizations 6000 and 5000. He received his BS from the University of Vermont and his PhD from the Deptartment of Hydrology and Water Resources at the University of Arizona – probably the leading hydrology program in the world. Darin is based in Organization 6300 where he initially enhanced the efforts of Sandia's Water Initiative - in particular basin-scale modeling of water balances in the southwestern US and potentially climinate change modelling. The expectation is that remote sensing/national security applications of his cosmic-ray work would be pursued as well. These interactions will extend outside of Organization 6000 and would be expected to involve greater interaction with Organization 5000. He joined Sandia in December 2007.

Progress reports on all six independent research projects follow.

Piezoelectric Properties of Arrayed Nanostructures of Zinc Oxide for Sensor Applications

David Scrymgeour (Org. 1725)
Truman Fellow

Project Purpose

The purpose of this work is to characterize the piezoelectric and electrical properties of individual nanostructures and the measurement of high-frequency impedance characteristics of both arrays and individual nanostructures. The piezoelectric effect combined with the small geometries of nanostructures gives an intrinsically high-frequency resonant behavior. These features can be exploited to create sensors that have the advantage of enhanced sensitivity due to higher operating frequency and smaller surface area. However, the basic properties of nanoscale piezoelectric structures must first be understood to implement such devices; building this understanding is the goal of this work.

Accomplishments

We successfully examined the resistivity of a population of ZnO nanorods through conductive atomic force microscopy (CAFM). We found that ohmically contacted nanorods show a wide resistivity distribution between 0.3 and 30 Ω·cm. This variation mirrors the previously measured piezoelectric effect that ranged from 0.67 to 8.75 pm/V among rods grown at the same time on the same sample. We directly tied the observed variation in piezoelectric coefficient to the variation in the conductivity of the individual rods by using correlated piezoelectric force microscopy and CAFM and found that high resistivity correlates to high piezoelectric response.

Additionally, we performed impedance spectroscopy measurements to characterize the high-frequency impedance properties of these nanostructured arrays. The transmission and reflection scattering parameters of both arrays and individual nanorods were measured from 0.1 to 50 GHz at room temperature. The scattering parameters determined the capacitance and resistance of the metal-nanowire contact and the intrinsic nanowire resistivity of individual rods. The calculated contact capacitance value per rod is ~10–16 F, consistent with a dielectric rod over a conducting plane. The average resistivity of nanowires is of the order of ~ 10^{-2} Ω·cm indicating the rods are intrinsically highly doped. Biasing the nanorods arrays caused a reduction in the contact resistance, which validated the fit of the data to a simple three-element circuit model. The unintentional preferential deposition of low-resistivity rods, and hence low piezoelectric coefficient, has precluded the observation of resonant behavior to date. This indicates that better control of the semiconducting properties during growth is needed before this material can be used as a high-frequency resonator.

Significance

By focusing on multiple property measurements of a large population of individual nanorods, we were able to determine that individual nanowire properties vary greatly. This makes the determination of material properties from either the extrapolation from a small number of measurements on individual nanostructures or from ensemble measurements of a large population prone to error. Additionally, the strong variation and interdependence of material properties — piezoelectric and electrical — is due to unintentional defect incorporation during nanomaterial growth. Until growth of nanostructures can be better controlled, wide variations in material properties will plague nanomaterials and limit their technological integration.

Refereed Publications

D.A. Scrymgeour and J.W.P. Hsu, "Correlated Piezoelectric and Electrical Properties in Individual ZnO Nanorods," *Nano Letters*, vol. 8, pp. 2204-2209, August 2008

Three-dimensional Analysis for Nanoscale Materials Science

Ilke Arslan (Org. 8625)
Truman Fellow

Project Purpose

The purpose of this project is to understand the fundamental properties of materials at the nanoscale, in both two and three dimensions through the development and application of advanced techniques in the transmission electron microscope. This fundamental understanding will lead to the design and fabrication of better devices and thereby advance technology. The materials tasks that were focused on in FY 2008 are materials for applications in hydrogen storage and electrical energy storage.

Accomplishments

The first completed task was on cobalt-based Fischer–Tropsch systems, which are widely used to convert synthesis gas to clean hydrocarbon fuel. Two Co_3O_4 catalyst systems with different supports were studied. We found that the first catalyst formed an interlocking structure with no free surface area. The second catalyst was more selective, and this was attributed to its unique nanocage morphology that allows larger surface area for reactions to take place. This 3D nanoscale information could not be quantified without the

use of scanning transmission electron microscope (STEM) tomography.

The second completed task was on GaN/AlN core/shell nanowires, which are important for light emitting diodes, diode lasers, and high electron mobility transistors. The surfaces play an important role in these 1D systems, and the only way to analyze the surfaces and bulk simultaneously is by using STEM tomography. While the defects seen in the 2D images appeared to be bulk defects, the 3D reconstructions revealed that the defects actually occur only on the surface of the nanowires.

The third completed task revolved primarily around technique development. It correlated electron tomography (ET) and atom-probe tomography (APT), which are both 3D techniques on the nanoscale. ET provides larger-scale morphological information while APT provides smaller-scale chemical information in 3D. Correlating these two techniques can yield a level of materials understanding that has never been reached before. This first correlation has allowed us to quantify the artifacts in both techniques, understand the evaporation process in APT, determine the optimal reconstruction parameters for both techniques, and evaluate the quality of the ET and APT reconstructions.

Significance

The impact of this project will help to enable technologies to meet the future energy needs of our Nation. In order to make our current energy materials more efficient and to develop new materials for future energy applications, fundamental structure-property relationships must be established on the nanoscale. Electron microscopy is one of the most important tools to meet this demand, and the quantitative 3D imaging and analysis developed in this project will play a vital role in moving our Nation's energy needs forward quickly and competently.

Refereed Publications

I. Arslan, J.C. Walmsley, E. Rytter, E. Bergene, and P.A. Midgley, "Toward Three-dimensional Nano-engineering of Heterogeneous Catalysts," *Journal of the American Chemical Society*, vol. 130(17), pp. 5716-5719, April 2008

I. Arslan, A.A. Talin, and G.T. Wang, "Three-dimensional Visualization of Surface Defects in Core-shell Nanowires," *Journal of Physical Chemistry C*, vol. 112(30), pp. 11093-11097, July 2008

I. Arslan, E.A. Marquis, M. Homer, M.A. Hekmaty, and N.C. Bartelt, "Towards Better 3-D Reconstructions by Combining Electron Tomography and Atom Probe Tomography," to be published in *Ultramicroscopy*

Passive and Active Electromagnetic Frequency Selective Surfaces for High-power Beam Applications

Hung (Jacques) Loui (Org. 5345)
Truman Fellow

Project Purpose

The purpose of this project is to create novel, reconfigurable, metal/dielectric surfaces/volumes for adaptive control over electromagnetic scattering. The idea is to embed tunable devices into the periodic unit cells of a thick metal plate, so that, collectively, the structure can affect electromagnetic beam propagation based on electrical configuration. Ferrite, a low-loss gyromagnetic material, exhibits a permeability tensor that is tunable via magnetic bias and can act as an absorber, phase changer, polarization converter, and reflector of electromagnetic excitation. The proposed design embeds ferrite rods and inductive coils inside the perforations of a hollow metal plate.

Accomplishments

In order to design and build tunable ferrite-embedded frequency selective surfaces (FSSs), electromagnetic properties of the ferrite used must be characterized. Although analytical forms of the permeability tensor exist for ferrite biased to saturation, they are not readily available for partially magnetized ferrite, a state important to the tunability of ferrite-embedded FSSs.

We discovered, through analysis and simulation, that the empirical model based on existing experimental data for partially magnetized ferrite did not match classical models as the ferrite becomes fully saturated. This fact requires experimental validation. Due to the lack of analytical, experimental, and manufacturing data on the gyrotropic permeability tensor of partially magnetized ferrite in the millimeter wave regime, we designed, analyzed, and constructed an experimental apparatus to provide measured permeability tensor needed by analysis tools. Technical features of this experiment important to making ferrite-embedded FSSs are as follows: (1) The experiment uses magnetic coil configurations similar to those used inside a FSS unit-cell; (2) Compact differential orthomode transducers provide high isolation between orthogonal ports for measuring material dispersion through Faraday rotation. Calibration and measurement of physical samples are under way.

COMSOL, a multiphysics software package was purchased and used in the analysis of waveguide structures partially filled with magnetized ferrite. Numerical results demonstrated tunable dispersion behavior in the unsaturated regime.

We continued construction of the Gaussian beam measurement setup for characterization of FSS. We designed a custom lens, holders, and sample fixtures. We also developed 3D ray-tracing software using the MATLAB language to design aspherical microwave lenses. We simulated a corrugated feed horn and lens combination (an electrically large problem) using CST Microwave Studio and showed that the feed horn's input match has < 1.5 voltage-standing-wave-ratio over the entire K-band in the presence of the lens, and that edge diffractions from the lens rim are minimal.

Significance

This approach overcomes material complexities and increases the likelihood of miniaturization success. This work has application to low-observable radio frequency antenna systems for defense applications, as well as applications in covert antenna systems and radar cross-section modification. This work is also appropriate for the development of active array antennas, which are relevant to synthetic-aperture radar, remote sensing, and nonproliferation applications.

Network Design Optimization of Fuel Cell Systems and Distributed Energy Devices

Whitney Colella (Org. 6339)
Truman Fellow

Project Purpose

This work involves the modeling of energy systems with the aim of designing them to achieve environmental, infrastructure security, and economic goals. Designs of alternative vehicles, power plants, and building thermal management systems, along with each technology's related energy supply chain, are being evaluated. For example, models test building energy demands against energy supplied by distributed cogenerative fuel cell power plants. Assessment criteria for these energy systems and supply chains include the following: (1) their impact on the environment; (2) their implications for national security; and (3) their costs to consumers, governments, and incumbent energy suppliers.

Accomplishments

This research analyzes alternative energy systems for their impacts on the environment and costs. Historical databases describing emissions from current energy generators are crosschecked and the rectified data are used to benchmark emissions from alternative technologies. Computer simulations are used to examine innovative designs for stationary polygenerative fuel cell power plants tuned to the electricity and thermal demand curves of the buildings they could serve. Model analyses are enabling evaluation of the energy supply by fuel cell systems and distributed energy devices relative to the energy demand in surrounding buildings. This work is achieving the following specific accomplishments.

1. Rectifying inconsistencies in historical emission accounting;
2. Quantifying and visualizing the change in emissions over time with a switch to alternative generators;
3. Building models that describe the behavior of individual energy systems; and
4. Analyzing distributed energy systems not just against electricity demand but also against thermal demand curves.

Results are being documented in refereed publications and in presentations at conferences.

Significance

This research supports key DOE environmental and energy efficiency missions. It supports the goals of the Energy Efficiency and Renewable Energy (EERE) Office, the Office of Electricity Delivery & Energy Reliability (OEDER), the Office of Fossil Energy, and the Hydrogen Program, by enabling fuel cell technologies for distributed stationary power, more-efficient fossil energy systems, reduction in carbon emissions, diversified energy supplies, modernized energy infrastructure, and optimal use of energy resources, with limited environmental impacts.

Refereed Publications

W.G. Colella, S.H. Schneider, and D.M. Kammen, "Mitigating Global Warming with Stationary Fuel Cell Systems: A Case Study of California," American Society of Mechanical Engineers (ASME), *Proceedings of the American Society of Mechanical Engineers (ASME) Second European Fuel Cell Technology & Applications Conference*, 2007

W.G. Colella, S.H. Schneider, D.M. Kammen, A. Jhunjhunwala, and N. Teo, "Part I of II: Development of Meress Model — Developing System Models of Stationary Combined Heat and Power (CHP) Fuel Cell Systems (FCS) for Reduced Costs and Greenhouse Gas (GHG) Emissions," *Proceedings of the 6th International Fuel Cell Science, Engineering & Technology Conference*, 2008

W.G. Colella, S.H. Schneider, D.M. Kammen, A. Jhunjhunwala, and N. Teo," Part II of II: Deployment of Meress Model — Designing, Controlling, and Installing Stationary Combined Heat and Power (CHP) Fuel Cell Systems (FCS) to Reduce Costs and Greenhouse Gas (GHG) Emissions," *Proceedings of the 6th International Fuel Cell Science, Engineering & Technology Conference, 2008*

Cosmic-ray Hydrometrology for Land Surface Studies

Darin Desilets (Org. 6312)
Truman Fellow

Project Purpose

The purpose of the project is to develop a passive and noninvasive method for measuring snow water equivalent and soil water content.

Accomplishments

We developed calibration curves and correction factors that allow cosmic-ray neutron intensity measurements to be used as a proxy for soil water content. The calibration function is applicable to a wide range of silica-dominated soils where vegetation is minimal. We have also developed calibration functions for vegetated terrain have. We have conducted measurements and neutron flux modeling work, with the aim of quantifying the sample volume represented by cosmic-ray neutron measurements.

Significance

One of DOE's principle goals is to ensure a reliable, affordable, and environmentally sound energy supply for our nation. The ever-increasing demands placed on available energy and water supplies coupled with the complex interdependencies relating these resources could threaten the continuity of energy supply in the future. The proposed project will develop tools and techniques that will be crucial to accurately understanding and predicting the availability of water for energy production and the myriad of other competing uses of this precious resource.

Multiscale Schemes for the Predictive Description and Virtual Engineering of Materials

Anatole von Lilienfeld (Org. 1435)
Truman Fellow

Project Purpose

This project's purpose is to assemble relevant techniques for virtually designing chemical compounds using multiscale simulation schemes. We have initiated work on various important aspects, including work on the accuracy of underlying first-principles methods, on randomly generated hydrocarbons, on electronic excitations for varying compounds, on alchemical derivatives of reaction barriers, and on improving thermodynamic properties of heat transfer fluid candidates.

Accomplishments

In collaboration with New York University, we furthered the molecular grand-canonical ensemble (MGCE) density functional theory (DFT) scheme, and we derived equations of motion in the elementary particle space of protons (defining atomic numbers) and electrons, the corresponding partition function, the incompressible phase-space volume element, and a Nose-Hoover chemostat.

In collaboration with Eidgenössische Technische Hochschule (ETH, Swiss Federal Institute of Technology) Zurich, we researched the prediction of molecular crystal structures. We concluded that the employed level of theory for computing interatomic forces — Kohn-Sham (KS) DFT augmented by London dispersion corrected atom-centered potentials — was insufficiently accurate when combined with a hybrid of genetically generated geometries/geometry relaxation or simulated annealing.

Further analysis of KS-DFT showed strong errors of interatomic many-body van der Waals forces in gas and bulk. This work was done in collaboration with the Fritz-Haber Institute, Berlin.

In collaboration with the Max-Planck Institute Mainz, we successfully generated randomized aromatic hydrocarbons with variable number of atoms or beads, a first step toward the subsequent residual current device (RCD) of Marcus-theory derived charge mobilities in liquid crystals.

Excitation energies from time-dependent DFT correlate well with the band-gap, using the same exchange-correlation potential, for all the neutral and cationic mutants of B and N doped benzene derivatives. This work represented collaborations with Ecole Polytechnique Federale (EPF), Lausanne.

In collaboration with University of Texas at Austin, we implemented alchemical derivatives, from the MGCE, into VASP and tested them for chemical reactions.

Accurate melting point calculations, using thermodynamic cycles, of heat transfer fluids were implemented and performed with the University of Notre Dame using LAMMPS (Sandia's molecular dynamics code).

Significance

The intended demonstration of solving the problem of compound design will serve to benefit Sandia science and mission areas that are involved with engineering material properties.

Refereed Publications

A. Tkatchenko and O.A. von Lilienfeld, "Popular Kohn-Sham Density Functionals Strongly Overestimate Many-body Interactions in van der Waals Systems," *Physical Review B, vol. 78, p. 045116-1-6, July 2008*

O.A. von Lilienfeld and P.A. Schultz, "Structure and Band Gaps of Ga-(V) Semiconductors: The Challenge of Ga Pseudopotentials," *Physical Review B*, vol. 77, p. 115202, March 2008

Two individuals were selected as Truman Fellows beginning October 2008. Abstracts of their planned research for FY09 follow.

Interfacial Electron and Phonon Scattering Processes in High-powered Nanoscale Applications

Patrick Hopkins (Org. 1513)
Truman Fellow

Dr. Hopkins' research is focused on understanding the physics of heat transfer in nano structures and development of measurement techniques to characterize heat transfer at material boundaries in these materials. The objective of the proposed research is to study heat transfer processes around structurally imperfect regions at interfaces in both traditional and novel thermal interface materials. The results of Patrick Hopkins' proposed research could have significant impact on the continued development of innovative devices and materials at Sandia and in U.S. industry. Patrick has degrees in mechanical engineering and physics and a minor in applied mathematics from the University of Virginia. He has an extensive list of publications and awards. Patrick joined the Microscale Science and Technology organization (1513) in August 2008.

Abstract

A significant limiting factor in next generation nanoelectronic systems is the large heat fluxes generated from operation. Inadequate power dissipation capabilities in these systems result in self-heating and increased operating temperatures that degrade device gain and efficiency and shorten device life. The materials used in the design and construction of the nanoelectronic devices and the dissipation of the heat from these devices contributes to overheating. Nowhere is this problem more pronounced than in high-powered systems, such as modern weapon, sensor, and signal processing systems and energy conversion systems, such as thermoelectric coolers and power generators. Therefore, thermal management in current and future nanoelectronic systems is a growing concern. As these nanoelectronic systems continue to decrease in characteristic sizes, the thermal management issues arise at the interfaces or junctions of different materials where energy carrier scattering is prominent. The key to thermal engineering of next-generation nanosystems is to understand the intrinsic properties of materials that affect interfacial thermal transport.

The objective of this proposed work is to study heat transfer processes around structurally imperfect regions at interfaces involving both traditional and novel nanostructures used in high-powered nanoelectronic and energy conversion applications. Deposition, fabrication, and post possessing procedures of nanocomposites and devices can give rise to interatomic mixing around interfaces of materials leading to stresses and imperfections that could affect heat transfer. As nanoapplications continue to decrease in characteristic sizes, the degree and depth of the interatomic mixing can be on the same order or greater than the sizes and length scales of the individual materials comprising the device. An understanding of the physics of energy carrier scattering processes and their response to interfacial disorder will elucidate the potentials of applying these novel materials to next-generation high powered nanodevices and energy conversion applications.

Development and Characterization of 3D, Nano-Confined Multicellular Constructs for Advanced Biohybrid Devices

Bryan Kaehr (Org. 1815)
Truman Fellow

Dr. Kaehr's research involves a new and unique technology for building almost any structure with proteins. Bryan developed his own research program in optical molecular biology and developed a new technique for making arbitrary, three-dimensional structures of proteins using multiphoton excitation to cross link proteins. The uses for these three-dimensional protein structures are only now being explored and the possibilities seem groundbreaking, from studying cell signaling to immobilization of a living cell to new sensor technologies based on living cells. Bryan's research impacts nano technology, microfluidics, sensors, cell signaling and photo-polymerization. Bryan Kaehr received his BS from the University of New Mexico (double major in Psychology and Sociology with a minor in biology) and PhD in Biochemistry at UT-Austin. His research has appeared in Scientific American, C&E News, and Biophotonics. He is first author on six papers and has been contacted by venture capitalists to explore possibilities for the new protein structure technologies he has developed. Org. 1815, Ceramic Processing and Inorganic Materials, became his host organization in August 2008.

Abstract

Inspiration for the design of new materials and devices is increasingly found in biological systems where sensitive detection, energy conversion and molecular/nano machinery have been continually improved upon by evolution. To impart the useful properties of biological systems into devices requires new ideas and technologies. Although there has been much focus on material functionalization using biomolecules, incorporation of self-sustaining and self-replicating components (e.g., cells, tissues and organisms) into solid-state platforms has received scant attention. Outside of native and well-controlled environments, cells are fragile and cell behavior is difficult to manipulate into complex systems such as tissues. In order to bridge the organic structures and functionalities of cells to the inorganic, solid-state materials of modern devices, functional biotic/abiotic interfaces are required. The proposed research will take advantage of recently developed strategies that allow the cell-directed assembly (CDA) of nanomaterials to form functional bio/nano interfaces (Baca et. al., Science 2006). This approach is an important step toward building solid-state devices that are enabled by cellular functions. Devices for sensing and computation will be further facilitated if higher order cellular functions, such as differentiation and intercellular communication can be maintained and exploited in biohybrid materials. Recent breakthroughs in 3D microfabrication that enable the topographical and chemical microenvironments of developing cell populations to be precisely defined (Kaehr & Shear 2007) will be employed to direct bio/nano interfaces to multicellular constructs. Patterning of multicellular constructs that can direct assembly of nano-structured films combined with the emerging tools of cellular (re)programming (i.e., synthetic biology) will permit the design of communication networks between engineered cell populations — enabling the development of cell-based circuitry. Incorporation of cellular functions into integrated micro-platforms will be facilitated and may allow the development of new technologies including cell-powered robots and “personalized” bionic implants.

SANDIA-UNIVERSITY RESEARCH PROGRAM [SURP]

Since 1958, Sandia National Laboratories has provided research-funding support to beginning faculty researchers at the University of New Mexico (UNM), the New Mexico Institute of Mining and Technology (NMT), and New Mexico State University (NMSU) through the Sandia-University Research Program (SURP). Each university researcher is partnered with a Sandia collaborator to satisfy the program's primary goals of obtaining needed scientific knowledge and technical expertise while strengthening the university-laboratory technical community in mission-relevant areas. Investment in new faculty development helps create partnerships that build long-term strength in areas deemed critical to support Sandia's Nuclear Weapons mission and its Science and Technology Research Foundations.

Funding for SURP comes from the U.S. Department of Energy/National Nuclear Security Administration's Office of Defense Programs through Sandia's Nuclear Weapons Strategic Management Unit (NWSMU). This program is currently part of the Nuclear Weapons Readiness in Technical Base and Facilities People Readiness workforce development portfolio. In order to ensure a close association between the faculty member and the Sandia technical collaborator, the SURP program has a matching-funds requirement for each funded research project. The Sandia collaborators view these investments as excellent leverage for their program's research dollars. A new award is $40,000 per project, with $15,000 coming from the Sandia collaborator.

The SURP projects are selected for their high relevance to Sandia's research interests and mission needs. The project should complement Sandia's Nuclear Weapons Capabilities as well as its Research Foundations, which include materials and process sciences, computational and information sciences, microelectronics and photonics, engineering, and pulsed power. Projects may also include maturation and/or commercialization research support of technologies under development at Sandia. SURP benefits to Sandia include increased understanding in the subject matter explored by the projects, exposure to unique research areas, cost-effective research, and collaborative relationships between Sandia and New Mexico university faculty.

Universities and individual faculty members benefit from their participation in SURP through increased interaction with Sandia researchers, increases in faculty research production, faculty and student recruitment, grants from other institutions, experience in managing projects and student assistants, and awards, tenure, and fellowships.

While Sandia selects SURP projects based on their value to Sandia's mission-relevant research needs, the Labs also tracks the significance of the SURP projects by their contribution to the broader scientific and technical communities. Two indicators of this significance are the additional funding and follow-on work obtained by the university researchers as a result of the SURP project and the number and breadth of conferences and publications that accept SURP project-related presentations and articles. A broad collection of national and international scientific and technical organizations and journals has accepted submissions related to the SURP projects by the university researchers. The diverse fields of these organizations represent Sandia's far-reaching interests and influence.

During FY2008, a decision was made by the NWSMU to scale down the program to consider second-year proposals only for FY2009, and to discontinue the program altogether in FY2010 and beyond. These decisions were made due to decreases in NW program funding.

An Augmented-reality Display System for Visualization and Training

Pradeep Sen
University of New Mexico

Carl Diegert (Org. 1412)
Sandia Principal Investigator

Abstract

A novel paradigm for interaction and visualization for complex data sets was proposed. Specifically, we built on the idea of *spatially aware computing*, in which a 3-D model in the computer's memory is mapped into our physical space through a user-specified transformation. During visualization, the motion-capture system registers the position of the user(s) as well as the position and attitude of a hand-held liquid crystal display (LCD) that is held and maps to the correct position in the model. The image displayed on the screen reflects the correct view for the user(s) as if they were standing in front of the model. In other words, the LCD display acts like a "window" to the virtual model stored in the computer. This interface allows us to visualize data in a more effective way than with conventional displays.

Accomplishments

In the first eight months, we have already accomplished many of the tasks described in the initial proposal and are well on our way to successful completion of the proposed work. We summarize our accomplishments below.

Milestone 1 – Acquisition of Parts and Equipment

We have acquired the necessary equipment for the construction of our system. This involved the purchase of the static workstation for rendering, several hand-held displays for user interaction, and other miscellaneous equipment and supplies such as a shutter or polarized glasses, motion-capture markers, cables or wireless video transmitters, etc. These items were all purchased with funds belonging to the PI and collaborators that are external to this project.

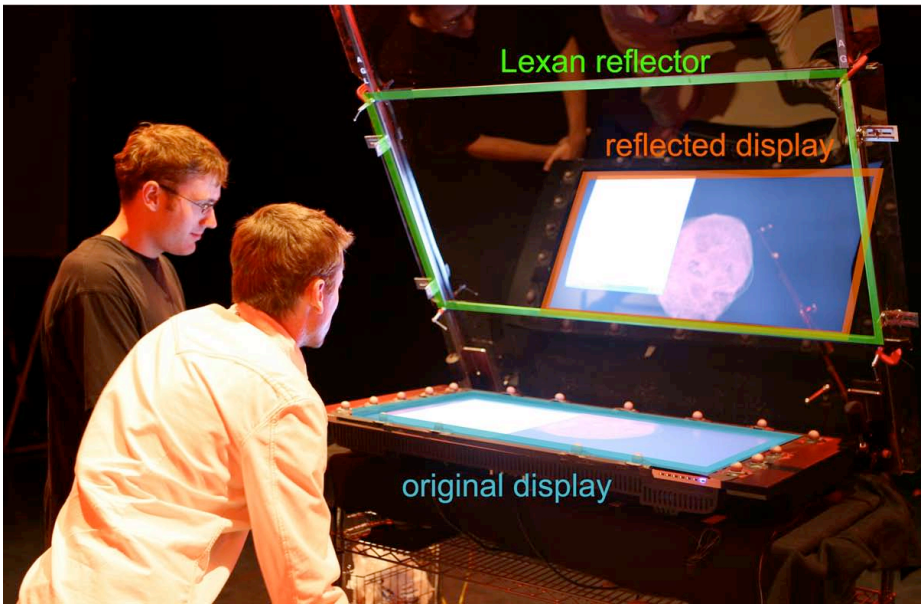


Figure 1. Augmented Reality Heads-up-display (AR HUD). As part of this project, we built a transparent heads-up-display to superimpose our rendered images onto real objects. The display itself is tracked by the motion-capture system so it can be moved around the scene. This means that the AR HUD is yet another "virtual window" that can be used by scientists when viewing their data sets. Here, two users view a medical data set through the AR HUD.

Milestone 2 – Development of Software Infrastructure

Once the equipment had been purchased, we developed the rendering infrastructure that uses the motion-capture information to generate the images that will be sent to the user displays. This was one of the more ambitious milestones since it involved significant development and engineering of the hardware and software integral to the system. The rendering system needed to be flexible enough to handle data from various sources, (e.g. from a vowel-based physical simulation or a set of 2-D image slices representing medical data). In addition, the workstation we secured needed to be able to transmit the image data to the hand-held displays for viewing. We spent considerable time debugging the system and then fine-tuning it to minimize the interaction latency. Most of our effort for the development of the system happened at this stage.

Milestone 3 – Initial Experimentation with System

Once the system was built, we began initial experimentation of the user interface on simple data sets such as the ones from the National Institutes of Health (NIH) Visible Human Project. Specifically, we used data sets of the brain and of a beating heart to demonstrate a proof-of-concept of our ideas. At first, the system was used only by the development team while we fixed major interface issues, refined the calibration procedure, etc. Results from these tests are shown throughout this proposal. The system is now ready for further testing with

our collaborators from Sandia and the Mental Illness and Neuroscience Discovery (MIND) Institute.

To help meet these three milestones, the PI's graduate student extended the initial prototype into a flexible system that can do spatially aware rendering based on the position of the display and the user as determined by the Vicon motion-capture system (milestones 1 and 2). Our system supports different rendering modes (e.g., volume rendering, standard OpenGL-style geometry-based rendering, and image-based rendering) which are useful for viewing different kinds of data sets. We have also purchased equipment using startup funds to develop different hand-held displays that allow the user to interact with the data. The key idea is that these displays can be interchanged seamlessly and our software is flexible enough to handle different devices and calibration procedures for each. Therefore, if a user wants to work with a particular display, they can simply add it to the system and our framework will automatically handle it.

We also have built an Augmented Reality heads-up-display (AR HUD) (Figure 1) which acts as a transparent, see-through version of the virtual window. The AR HUD consists of a metal frame on wheels upon which a piece of thin Lexan transparent plastic has been suspended. A flat-panel display is placed horizontally on the surface below the Lexan, which is reflected by the plastic to create a see-through floating version of the display. This allows us to superimpose rendered images onto real objects, giving a better sense of spatial location in the data. Several of the images shown in this proposal are taken through our AR HUD in order to superimpose the data onto real objects (Figures 2 and 3). Since the SURP award does not provide funds for hardware, we designed the system to cost less than one hundred dollars and borrowed the remaining equipment (e.g., the flat panel display and the PC to drive it).

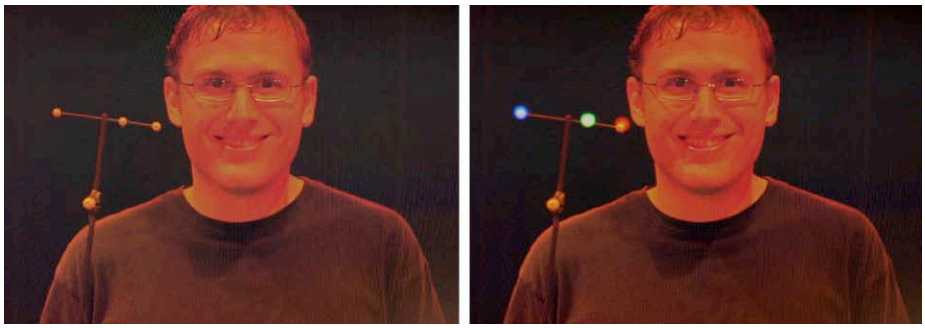


Figure 2. Demonstration of calibration using the AR HUD. After our calibration procedure, the rendering system has accurate information regarding the positions of the display and the viewer and can therefore render synthetic objects accurately through the "window." Here, we photograph a user holding a wand through the AR HUD. Since both the camera and the AR HUD have been calibrated, the system can place the colored dots (right) accurately on top of the wand's three markers as seen by the camera. The correct alignment can be seen from any viewpoint and indicates that virtual objects (e.g., a brain, heart, etc.) will properly align to real world objects (e.g., the patient's body).

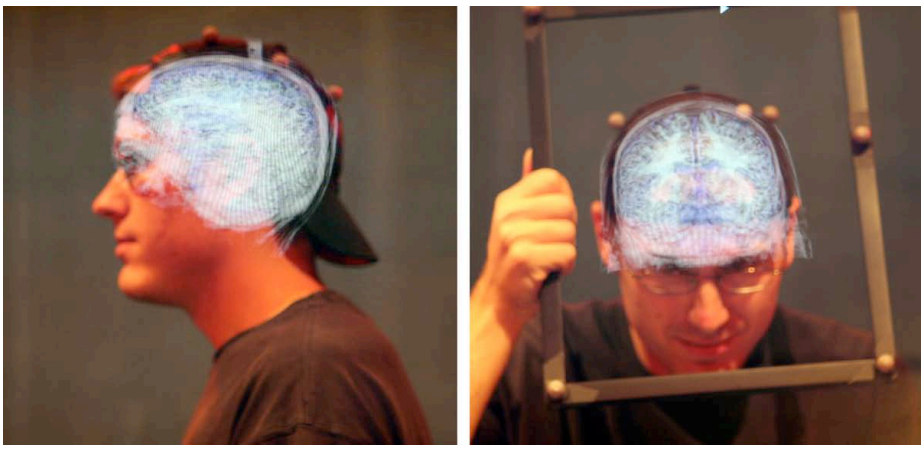


Figure 3. Visualization of brain data sets. On the left, we visualize a brain data set that has been registered to a "patient's" head. This allows us to visualize the data set in a more intuitive manner than if we looked at it on a standard 2-D display. For example, this interface allows the doctors to see the brain in exact relationship to the patient's head. As the patient moves his head, the brain moves accordingly, therefore providing an intuitive way to rotate and manipulate the data set. On the right, we place the slicing prop halfway through the brain to create a visible slice. Both of these images have not been manipulated and are what the user would see through the AR HUD.

Significance

After the system was built and the individual applications developed, we began to experiment with the user interfaces (milestone 3). One of the main engineering challenges we had to overcome in this phase of the project was the accurate calibration of the system in order to achieve reliable results. After all, the virtual window paradigm relies on the fact that the rendering system knows the position of both the window and the viewer to a high degree of accuracy in order to generate images with the correct perspective. Initially, when our system was not calibrated, the mismatch between the rendered images and reality was distracting. However, once we calibrated the system (which was particularly important for the AR

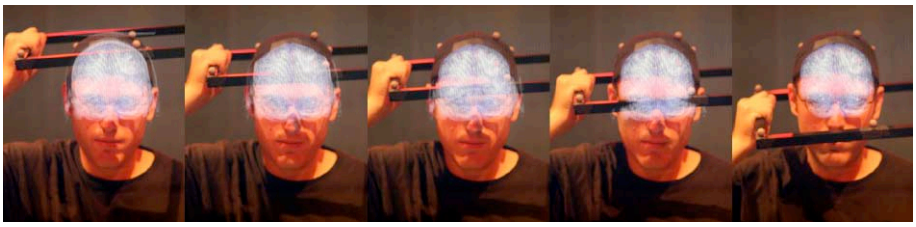


Figure 4. Interactive visualization. In this example, we simulate the removal of skull to reveal the brain by moving the slicing prop down across the patient's head.

HUD) the results were even more convincing. Figure 2 shows the view through the AR HUD after successful calibration.

The initial applications developed as part of milestone 3 were for medical visualization, which is of particular interest to the MIND Institute. Our system was able to register a data set such as a human brain to a person's head, providing a spatial context for the data. In addition, our experimentation with user interfaces led to the construction of a hand-held prop frame to allow the user to specify the cutting plane for AR HUD based applications. Examples of our system in action for medical visualization are shown in Figures 3 – 6.

Aside from the stated goals of developing the system and getting results with actual medical data, the current SURP proposal has also led to other accomplishments. The PI's student, Mark Waligora, who worked on this project, has written a Masters Thesis on this work entitled "Virtual Windows: Designing and Implementing a System for Ad-hoc Positional Based Rendering" and is graduating in May of 2008. We are also in the process of writing up our results in a paper ("Virtual Windows: A framework for spatially aware, ad-hoc visualization" by Pradeep Sen, Mark Waligora and Joe Kniss), to be submitted to the journal *IEEE Transactions of Visualization and Computer Graphics*.

Publications

P. Sen, M. Waligora, J. Kniss, "Virtual Windows: A Framework for Spatially Aware, Ad-hoc Visualization", I*EEE Transactions of Visualization and Computer Graphics Journal*, submitted

M. Waligora, "Virtual Windows: Designing and Implementing a System for Ad-hoc Positional Based Rendering", Masters' Thesis, May 2008

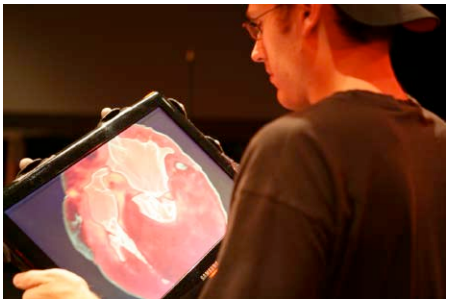
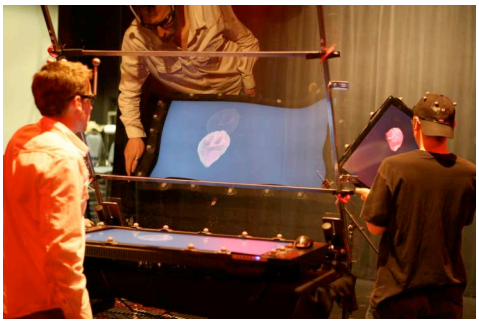
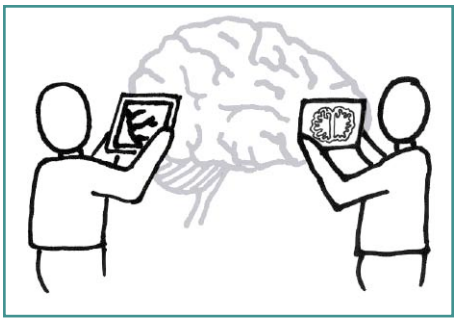


Figure 5. Using the virtual window to slice through a data set. Student Mark Waligora uses the screen to slice into a volume rendering of a beating heart. We find that spatial relationships are easier to understand using the spatially aware paradigm.

Figure 6. Multiple users interacting with the system. One of the key visions for the project was to enable multiple scientists to visualize complex 3D data in a collaborative manner. For example, the image on the left shows two researchers examining a beating heart data simultaneously through both the AR HUD and one of the hand-held displays. For reference, compare this image to the one on the right, which is taken from the initial SURP proposal. Thanks to the support from Sandia, that vision is now a reality.





An Advanced Security Policy Engineering Framework for Protecting Distributed and Critical Systems

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New Mexico Institute of Mining and Technology

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Abstract

Distributed computing will continue to play a critical role in national/global cyber infrastructure, and security services in distributed systems are strongly required. The problem we addressed was how to provide an advanced access control policy-engineering framework for distributed systems. Specifically, our focus was on developing a formal approach to modeling a distributed authorization, which can be used to analyze flaws in authorization. This research has broad impact by providing a key mechanism for better understanding the security challenges of, designing overarching security architectures for, and enabling formal specification and verification of an authorization service in distributed systems.

Accomplishments

The PI at NM Tech proposed a formal model of role-based distributed access control for better understanding and analysis of trust-based access control policies and mechanisms. The formal model is based on the least fixpoint approach. The approach, as shown in Figure 1, deals with how to model different types of authorization in a consistent manner by using a mathematical lattice structure, how to model different kinds of credentials by using a monotonic license function, and how to implement distributed access control enforcement engines by using the least fixpoint semantics.

$$
\begin{aligned}
&s \in Users\\
&e \in Permissions\\
&r \in Roles = LRole + TDRole\\
&\langle s,r\rangle \in UA = Users \times Roles\\
&\langle p,r\rangle \in PA = Permissions \times Roles\\
&\langle r',r''\rangle \in TA = (LRole \times TDRole)\\
&\langle r',r''\rangle \in RH = (LRole \times LRole) + (TDRole \times TDRole)
\end{aligned}
$$

$$
\begin{aligned}
&i \in Ident \;=\; Principal \rightarrow Users\\
&u \in Auth = Principal \rightarrow \mathcal{P}(Permissions)\\
&\quad UAssertion = Principal \times UA\\
&\quad RHAssertion = Principal \times RH\\
&\quad TAssertion = Principal \times TA
\end{aligned}
$$

$$
\begin{aligned}
&\mathcal{M}_{UALicense} : UA \times AuthMap \rightarrow Auth\\
&\mathcal{M}_{UALicense}(\langle s,r\rangle, m) = \lambda p'.\{e \mid i(p') = s \text{ and } \langle e = m(p)(p'),r\rangle \in PA\}
\end{aligned}
$$

$$
\begin{aligned}
&\mathcal{M}_{UAssertion} : UAssertion \rightarrow Assertion\\
&\mathcal{M}_{UAssertion}(p,\langle s,r\rangle) = \langle p, \lambda m.\{\mathcal{M}_{UALicense}(\langle s,r\rangle, m)\}\}
\end{aligned}
$$

$$
\begin{aligned}
&\mathcal{M}_{RHLicense} : RH \times AuthMap \rightarrow Auth\\
&\mathcal{M}_{RHLicense}(\langle r',r''\rangle, m) = \lambda p.\bigsqcup\{\exists\langle i(p),r\rangle \in UA,\\
&\quad if(r' \preceq r),\ then\ \mathcal{M}_{UALicense}(\langle s,r'\rangle, m)(p),\ \mathcal{M}_{UALicense}(\langle s,r''\rangle, m)(p)\}
\end{aligned}
$$

$$
\begin{aligned}
&\mathcal{M}_{RHAssertion} : RHAssertion \rightarrow Assertion\\
&\mathcal{M}_{RHAssertion}(p,\langle r',r''\rangle) = \langle p, \lambda m.\{\mathcal{M}_{RHLicense}(\langle r',r''\rangle, m)\}\}
\end{aligned}
$$

$$
\begin{aligned}
&\mathcal{M}_{TALicense} : TA \times AuthMap \rightarrow Auth\\
&\mathcal{M}_{TALicense}(\langle r',r''\rangle, m) = \lambda p.\bigsqcup\{\exists\langle i(p),r\rangle \in UA,\\
&\quad if(r' \Rightarrow r),\ then\ \mathcal{M}_{UALicense}(\langle s,r'\rangle, m)(p),\ \mathcal{M}_{UALicense}(\langle s,r''\rangle, m)(p)\}
\end{aligned}
$$

$$
\begin{aligned}
&\mathcal{M}_{TAssertion} : TAssertion \rightarrow Assertion\\
&\mathcal{M}_{TAssertion}(p,\langle r',r''\rangle) = \langle p, \lambda m.\{\mathcal{M}_{TALicense}(\langle r',r''\rangle, m)\}\}
\end{aligned}
$$

Figure 1. A mathematical approach to better understanding role-based distributed access control

The proposed model was extended so that it could handle non-monotonicity in license functions; monotonic licenses in the previous model could only lead to increase in the level of authorization given to a principal, and this caused significant limitation on its ability to express and analyze diverse access control policies and mechanisms. To express various types of restrictions in the model, new types of licenses were defined—negative licenses. Hence, license is a set of both negative licenses and positive licenses. Negative licenses can be used to express separation of duty constraints in role-based access control (RBAC). However, they can effectively represent other kinds of negativity in authorization assignment in the model. Simply put, the authorization expressed in a negative license is set disabled in the original *Auth* lattice so that the requesting principal can never obtain that authorization in the *Auth* lattice. This notion was incorporated into the previous model seamlessly, resulting in an extended model of understanding and analyzing distributed access control. The result of this research is being prepared for publication in security conference proceedings or journals.

Attributes in credentials used for distributed access control need to be protected not just from its integrity violation but also its privacy violation. The PI proposed an approach to enabling selective attribute sharing in distributed computing environments, thereby providing a better privacy mechanism in such environments. To support selective data sharing, an authenticated dictionary (ADT)-based credential was developed, so that it could allow a user to share only a subset of his attributes certified by other organizations. A security architecture was designed and proof-of-concept prototypes were implemented, along with performance testing. The results of this research were accepted for publication in security workshops (TrustCol 2007 and TrustCol 2008), and are also currently under submission (IFIP SEC 2009).

The PI at NM Tech and at Sandia proposed an approach to protecting sensitive data stored in directory services, which are commonly used to store information related to individuals, and often act as a source for security services, such as authentication and access control, in collaborative applications within/across organizations. Existing solutions offer minimal protection against insider attacks, a growing threat to both government and industry data services. The approach leveraged virtual directories and data encryption to provide a user-centric approach to data protection, delegation, and collaboration. A security architecture was designed and a proof-of-concept prototype was implemented, along with performance testing. The result of this research was accepted for publication in a security conference (CollaborateCom 2008).

One of the issues that the PI at NM Tech did not include in the submitted proposal but found important was privacy protection. Privacy protection is strongly required, not just in trust establishment in role-based distributed access control, but also in current federated identity-based networks. The notion of user-centricity has been proposed to help address this issue. The basic notion of user-centricity is to give users a larger degree of control over their attributes, thus providing an ideal mechanism for upholding user privacy. Therefore, the PI also investigated how to address this issue by proposing a user-centric approach to enabling selective data sharing in distributed computing environments.

Significance

A grant proposal based on the result of this research was submitted to the National Science Foundation (NSF) on December 10, 2007. The proposal was not awarded in full amount ($447,130). However, the PI, collaborating with Dr. Gail-Joon Ahn at Arizona State University, is currently waiting for the result of a small grant proposal submitted to NSF at the request of the program manager at NSF. If funded, the PI will continue the research on distributed access control and user privacy protection in distributed/federated environments.

Presentations

D. Shin and R. Lopes, "Enabling Interoperable and Selective Data Sharing among Social Networks Sites," in Proceedings of the 3rd International Workshop on Trusted Collaboration (TrustCol 08 - in conjunction with CollaborateCom 08), Orlando, FL, November 13, 2008

W. Claycomb and D. Shin, "Protecting Sensitive Information in Directory Service using Virtual Directories," in Proceedings of the 4th International Conference on Collaborative Computing (CollaborateCom 08), Orlando, FL, November 13-16, 2008

R. Lopes and D. Shin, "Controlled Sharing of Identity Attributes for Better Privacy," in Proceedings of the 2nd International Workshop on Trusted Collaboration (TrustCol 07 - in conjunction with CollaborateCom 07), White Plains, NY, November 12-15, 2007

Conference Proceedings

D. Shin, R. Lopes, and G-J. Ahn. "A Framework for Enabling User-controlled Persona in Online Social Networks," submitted to the 24th IFIP International Information Security Conference (SEC 2009)

Advances in Sensitivity Analysis for Complex Computer Models

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Abstract

The understanding of many physical and engineering phenomena of interest to Sandia involves running complex computational models. With problems of this type, it is important to understand the relationships between the input variables (whose values are often imprecisely known) and the output. The goal of sensitivity analysis (SA) is to study this relationship and identify the most significant variables affecting the results of the model. In this project, we have improved upon existing methods for SA of complex computer models. SA can now be carried out more efficiently, thus allowing for a better understanding and improvement of complex computer models.

Accomplishments

This project resulted in the development of algorithms and software to perform sensitivity analysis of computational models. Specifically, the methodology developed for sensitivity analysis builds on the idea of sensitivity indices calculated using variance-based decomposition (VBD). A sensitivity index is a measure of the variance of the response that is due to an input. The new ideas here focus on the use of meta-models (surrogate models, response surface models) to perform the variance-based decomposition, as well as using bootstrap sampling to calculate confidence intervals on the sensitivity indices. Thus, instead of simply producing a ranking of variables by their importance, the methods developed allow one to calculate a sensitivity index value (e.g., the index for variable 3 is .29, indicating that 29% of the uncertainty of the output is due to variable 3) as well as a confidence interval. If the confidence interval is small, for example [0.25, 0.35] with respect to variable 3, it indicates that the statistics for this problem are probably sufficiently resolved and the meta-models are adequate. If the confidence interval is large, for example [0.01 to 0.59] with respect to variable 3, this indicates that further investigation is warranted.

A software package in the R computing language was developed to implement the new SA methodology described in this report. The software package currently is called CompModSA. CompModSA has several meta-modeling techniques that the user can choose from to perform sensitivity analysis, including: linear, rank, or quadratic regression; local regression; projection pursuit or recursive partitioning regression; MARS (multivariate adaptive regression splines); ACOSSO (Adaptive Component Selection and Shrinkage Operator); and a Gaussian Process model. The software package also has several controls to allow for variable selection in the identification of important inputs, and to control the bootstrapping calculations which generate confidence intervals on the sensitivity indices.

Some example output from the toolkit is shown in Figure 1. In this problem, we had a seven-dimensional input space and we wanted to investigate

Figure 1. Demonstration results from the CompModSA software package

```
QUADRATIC REGRESSION

Output = V8

Fitting Model

surface = rs.reg
Stepwise Addition:
 Model              GCV Score
 5                  22.587
 5 3                 7.9086
 5 3 7               0.14212
 5 3 7 4             0.071457
 5 3 7 4 6           0.02461
 5 3 7 4 6 2         0.010122
 5 3 7 4 6 2 1       0.011912

Stepwise Deletion:
 Model              GCV Score
 5 3 7 4 6 2         0.010122
 5 3 7 4 6           0.02461
 5 3 7 4             0.071457
 5 3 7               0.14212
 5 3                 7.9025
 5                  22.587

Final Model: 5 3 7 4 6 2

Estimated Model Summary:
Model: V8 = f(V5, V3, V7, V4, V6, V2)
Rsq = 0.9999474
dfmod = 27

Input  S.hat  S.cum  T.hat  95% T CI        p-val
V5     0.772  0.772  0.780  (0.736, 0.828)  0.000
V3     0.153  0.924  0.138  (0.077, 0.166)  0.000
V7     0.070  0.994  0.072  (0.044, 0.094)  0.000
V4     0.006  1.000  0.000  (0.000, 0.021)  1.000
V6     0.000  1.000  0.000  (0.000, 0.018)  0.360
V2     0.000  1.000  0.008  (0.001, 0.015)  0.020
```

```
MARS
Output = V8

surface = mars

Estimated Model Summary:
Model: V8 = f(V5, V3, V7, V4, V6, V2, V1)
Rsq = 0.999999
dfmod = 69

Input  S.hat  S.cum  T.hat  95% T CI        p-val
V5     0.776  0.776  0.786  (0.743, 0.887)  0.000
V3     0.149  0.925  0.139  (0.085, 0.171)  0.000
V7     0.075  1.000  0.070  (0.000, 0.104)  0.040
V4     0.000  1.000  0.000  (0.000, 0.017)  1.000
V6     0.000  1.000  0.000  (0.000, 0.035)  1.000
V2     0.000  1.000  0.003  (0.000, 0.027)  0.280
V1     0.000  1.000  0.002  (0.000, 0.018)  0.400

ACOSSO
Output = V8

surface = acosso

Estimated Model Summary:
Model: V8 = f(V5, V3, V7, V4, V6, V2)
Rsq = 0.9998868
dfmod = 47.29244

Input  S.hat  S.cum  T.hat  95% T CI        p-val
V5     0.775  0.775  0.786  (0.730, 0.827)  0.000
```

the importance of these inputs on the output. Figure 1 shows three meta-models being fit to this data: Quadratic Regression, MARS, and ACOSSO. For each meta-model, the variables that are selected to be included in the meta-model are reported, along with their ranking by sensitivity index and be the confidence interval on the sensitivity index. Note that two sensitivity indices are reported: Si, which is the proportion of the variance in the output that can be attributed to variable xi alone, and Ti, which corresponds to the total uncertainty that can be attributed to xi and its interaction with other variables. In this example, quadratic regression identifies variable 5 as being most important, then variable 3, then variable 7, etc. The estimate of the T index (T.hat) for variable 5 from the quadratic regression model is 0.78, with a 95% confidence interval of [0.736, 0.828]. Similarly, the estimate of the T index for variable 3 is 0.138, etc. The estimate of the T index for variable 5 from the MARS model is very close to that estimated based on the quadratic regression model: it is 0.786, with a confidence interval of [0.0743, 0.887]. Finally, ACOSSO produces similar estimates for the sensitivity indices as quadratic regression and MARS. This particular data set is well fit by the meta-models, with R-squared values over 0.99 for all three meta-models. However, there are many cases when the data comes from highly nonlinear phenomena with discontinuities and/or noisy data. In these situations, one can use the CompModSA toolkit to investigate the efficacy of various meta-models and compare the sensitivity indices and rankings produced by several methods. This allows for better insight into the important variables and can help produce more robust answers.

A Sandia Report (SAND 2008-6570) containing the evaluation of new meta-models for SA and techniques for developing confidence intervals for SA measures has been completed. This report has been submitted for internal review and also has been submitted as a journal article to Reliability Engineering and System Safety. The CompModSA software package is described in this report.

We have completed a manuscript covering the Loco-spline methodology proposed in last year's SURP proposal. This work has been submitted to the Journal of the American Statistical Association the summer of 2008 and is currently in review. We have also completed a manuscript discussing the idea of a Bayesian variable selection and Smoothing Spline - Analysis of Variance (SS-ANOVA) structure for covariance in spatial models which was proposed in last year's SURP proposal. This work was sent to Technometrics for publication and has been accepted. In fact, the editors liked it so much they invited us to give a talk on this paper at the Joint Statistical Meetings (the largest statistics conference) in the summer of 2009. A book on sensitivity analysis is being written in collaboration with peers. This book is intended to be a reference primarily for practitioners of SA such as analysts at Sandia or similar institutions. We have finished writing several sample chapters and the book is on schedule for publication in the fall of 2009.

Significance

To our knowledge, bootstrap methods have never been used in conjunction with meta-models to compute confidence intervals on sensitivity indices in this way. The combination of meta-models plus bootstrapping can result in a highly efficient way to calculate sensitivity indices and their confidence intervals for very expensive computer models.

Papers

C.B. Storlie, L.P. Swiler, J.C. Helton, E.A. Baldwin, and C.J. Sallaberry, "Confidence Intervals for Sensitivity Measures Obtained with Nonparametric Regression Procedures," SAND Report 2008-6570. Also submitted to *Reliability Engineering and System Safety* (in review)

C.B. Storlie, H.D. Bondell, and B.J. Reich, "Locally Adaptive Smoothing Splines," *Journal of the American Statistical Association* (in review)

C.B. Storlie, H.D. Bondell, B.J. Reich, and H.H. Zhang, "Surface Estimation, Variable Selection, and the Nonparametric Oracle Property," *Statistica Sinica* (in review 2008)

B.J. Reich, C.B. Storlie, and H.D. Bondell, "Bayesian Variable Selection for Nonparametric Regression Models," *Technometrics* (accepted 2008)

B. Iooss, C.B. Storlie, H. Monod, and G. Pujol, "Sensitivity Analysis with R," *Springer Series: Use R* (to appear fall 2009)

Invited Lectures and Presentations

"Surface Estimation, Variable Selection, and the Nonparametric Oracle Property," Chinese University of Hong Kong, Hong Kong, China, April 2008

"An Efficient and Effective Procedure for Sensitivity Analysis of Complex Computer Models," Sandia National Laboratories Seminar, Albuquerque, NM, March 2008

"Confidence Limits for Sensitivity Indices Estimated via Meta-Models," Joint Research Commission Workshop, Ispra, Italy, February 2008

"The Adaptive COSSO for Nonparametric Surface Estimation and Model Selection," Los Alamos National Laboratory Seminar, Los Alamos, NM, November 2007

Development and Application of Modern Analysis Techniques to Determine Yields of Nevada Test Site Explosions Using Sandia Seismic Data

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Robert E. Abbott (Org. 1646)
Sandia Principal Investigator

Abstract

Many techniques have been developed to discriminate between an explosion and an earthquake and to determine the yield of explosions. Sandia has maintained the Leo Brady Seismic Network (LBSN) since 1960 to record nuclear tests at the Nevada Test Site, providing a unique data set of seismic waveforms for yield determination. We apply several existing techniques that measure size of a test; this is used as a proxy for actual yield. Two of the methods, both using the L_g-coda portion of the seismogram, perform better than the current method used by Sandia.

Accomplishments

Seismic magnitude (m) is proxy for test yield, where a larger magnitude indicates a larger yield. The magnitude measurements described below are similar because they use amplitudes (A) measured on a seismogram to estimate test size. The general magnitude equation form is:

$$m = log_{10} A + D$$

where D is a correction based on the source-receiver distance (SRD) so that magnitudes measured at different stations are equal. Subscripts are added to the m indicate which arrival amplitude was measured. Figure 1 shows a seismogram with phases identified.

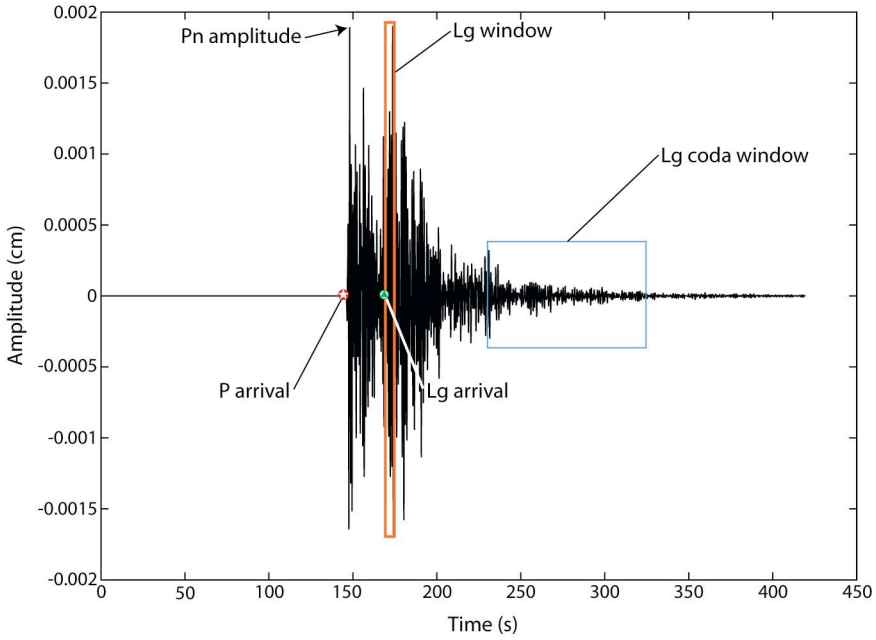


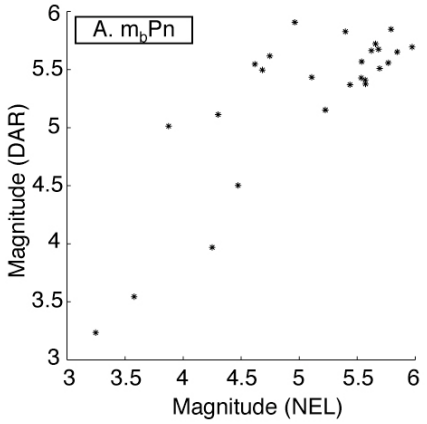
Figure 1. Seismogram from NTS UGT Tortugas recorded at station Darwin showing from where, on a seismogram, different data for the methods described below is derived. For the body-wave magnitude, $m_{b(Pn)}$, the amplitude pick would be the large peak after the first arrival of the energy. For $m_{b(Lg)}$, the rms-amplitude in the L_g-window was calculated. The L_g window is based on group velocities of 3.3 and 3.6 km/s. The L_g-coda window length is based on group velocities of 0.85 and 1.5 km/s. This window was used to calculate $m_{b(Lg\text{-}coda)}$ and the energy of the seismogram.

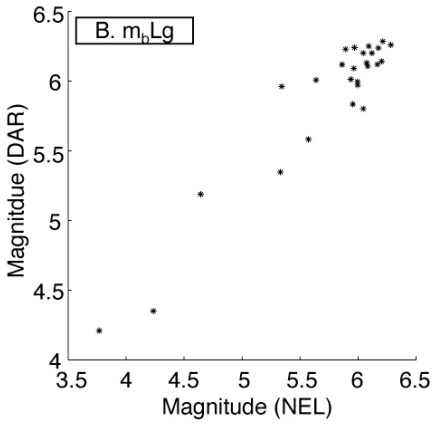
Body-wave magnitude measurements, $m_{b(Pn)}$ (Vergino and Mensing 1990), use the first-arriving energy (P) to estimate the size of the test (Figure 1). This method is most similar to Sandia's method for yield estimation, which also uses P energy. For each test, single station and network average magnitudes were calculated. Figure 2A plots $m_{b(Pn)}$ for two stations. The scatter indicates the method did not perform well – the magnitudes should be equal. This is either due to differences in the path traveled or because many stations have a small SRD.

The second magnitude measurement, $m_{b(Lg)}$ (Patton 1988), uses a later phase, L_g, to estimate test size (Figure 1). Patton (1988) tests two different techniques for measuring the amplitude of the L_g phase. Method one uses the third largest amplitude after the L_g arrival and method two uses the rms-amplitude of a section of the seismogram (Figure 1). We attempted both methods and preferred the second as it gave more consistent results (less scatter between the $m_{b(Lg)}$ at two different stations) and is easily automated. This method shows less scatter than $m_{b(Pn)}$ (Figure 2B).

The third magnitude technique uses an L_g-coda window (Figure 1) to measure the magnitude of the test (Mayeda 1993). The average amplitude of the window is used to estimate the test size. This method requires a digital waveform and is easily automated. The results are very stable (Figure 2C) and $m_{b(Lg\text{-}coda)}$ clearly performs best.

The amplitude spectrum of the seismogram is found by converting from the time domain to the frequency domain using a fast Fourier transform (FFT). The spectrum is fit for two





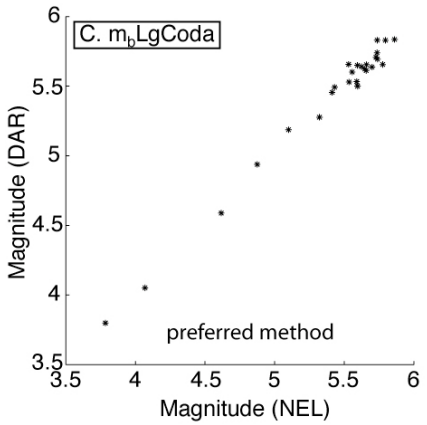


Figure 2. A comparison of magnitude measurements for 2 seismic recording stations in the Leo Brady Seismic Network (NEL = Nelson, NV, DAR = Darwin, CA). A. $m_{b(Pn)}$ does not perform well in most cases at predicting similar values for the same test at different stations. B. For $m_{b(Lg)}$ Darwin is almost always higher than the value at Nelson. Also, tests with magnitudes >5 still show scatter. C. The $m_{b(Lg-coda)}$ measurement is the most stable, and improves on previous methods used. The scatter for the tests with magnitudes >5.5 is much smaller.

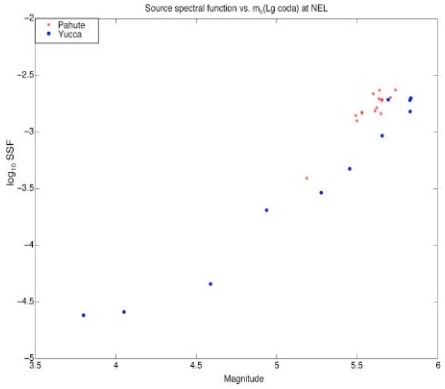


Figure 3. Plot of source spectral function (SSF) calculated on the L_g-coda window shown in Figure 1. The values for Pahute Mesa tests are larger than Yucca Flats tests due to differences in the geophysical parameters of the areas. If these parameters are improved this method will likely do as well as $m_{b(Lg-coda)}$ at predicting the size of a nuclear underground test.

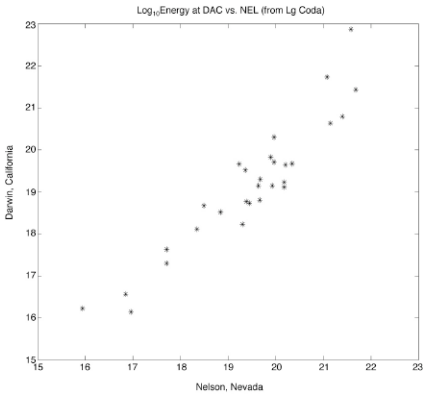


Figure 4. Plot of energy values calculated on the L_g-coda window shown in Figure 1. The values at Darwin are larger than those at Nelson likely due to input parameters. If these parameters are improved this method will likely do as well as $m_{b(Lg-coda)}$ at predicting the size of a nuclear underground test.

parameters, corner frequency and source spectral function (SSF) (Fisk 2007). The SSF is related to the size of the test. The results are promising; however, there is separation of test size dependent on location. This separation is not seen in any other techniques and is likely due to differences in geophysical parameters (Figure 3).

The seismic energy is measured by integrating a portion of the seismogram and correcting for source properties and path effects (Newman and Okal 1998). Estimates using both P and L_g-coda were attempted; results from the P-measurements were unstable. Figure 4 shows results using L_g-coda. While not as good as the $m_{b(Lg-coda)}$, it shows promise and could be refined by improving the input parameters.

Measurement methods using L_g-coda performed the best for all stations in the LBSN and are easily automated; $m_{b(Lg-coda)}$ is the preferred method. Computer programs for each method were delivered to Dr. Abbott.

Some of the methods that were initially proposed were not used because of problems using the first arriving phase, P. The arrival was problematic for two reasons: (1) The SRD for a majority of the source-station pairs is small enough that P_n and a different phase, P_g, arrive at the same time at nearly every station and (2) It requires a good model of the path effects for source receiver pairs. Developing such a model is outside of the scope of this project. Because it is not affected by path, we concentrated on methods that utilized the L_g and L_g-coda portions of the seismogram.

Significance

Because of the promising results of the study, the Sandia PI will be applying for funding in order to digitize older analog-tape seismograms so that the historic record can be improved. The greater seismological community will also be interested in having access to this data.

Publications

K.A. Schramm, S.L. Bilek, and R.E. Abbott, "Nuclear-Test Yield Determination of NTS Events Using Data from the Leo Brady Seismic Network," *Seismol. Res. Lett.*, **76**(2), 300, 2008

K.A. Schramm, S.L. Bilek, and R.E. Abbott, "Analysis of Modern Techniques for Nuclear-Test Yield Determination of NTS Events Using Data From the Leo Brady Seismic Network," *Eos Trans. AGU,* **88**(52), Fall Meet. Suppl., S43A-1058, 2007

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Design and Development of a Ku-band Planar Scanning Array Using Rotman Lens

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Abstract

The Advanced Instrumentation Systems Department at Sandia is responsible for the transmission and acquisition of data from a wide variety of complex test objects. Recent state-of-the-art test objects demand higher data rates with simultaneous use of tracking and data acquisition capabilities, thereby necessitating use of electronically scanned or phased array antennas with multi-directional pointing capabilities. There exist quite a few technologies, operating at radio frequency (RF), intermediate frequency (IF), digital and optical or hybrid thereof, and a number of ways that these could be used to accomplish a particular task at hand. Using RF beam forming, however, has the advantage of simplicity and lower cost with a potential to meet the demands for many applications. The RF beam former that utilizes a Rotman lens to feed a large number of array elements is considered a good scanning system both for multiple simultaneous beams and for scanning applications. Its use in microstrip form is highly appealing for both military and commercial applications.

This project is aimed at quantifying the performance parameters of a Ku-band planar scanning array using a Rotman lens. The primary objective is to select optimum technology, configuration and design parameters for a Rotman-lens-based antenna system that can meet Sandia's requirements of data transmission and acquisition. This objective is achieved using theoretical and simulation study of various Rotman-lens configurations. An optimum algorithm is developed to optimize various antennas design parameters. These parameters are then used as input for the simulation software provided by ANSOFT, a software company, to synthesize and analyze the antenna pattern and to generate performance parameters. The results of both theoretical and simulation studies are presented in this report. As a result of these studies, a scaled-down second bench-top prototype is under fabrication to demonstrate the feasibility and working of the system, and compare its performance results with those of simulations.

Accomplishments

Introduction

Modern communication systems often demand wide bandwidth, multiple beams, and beam steering capability. Multiple beam antennas that use beam switching offer a less expensive and compact alternative to traditional phased arrays requiring more complex fabrication. A multiple beam antenna has a capability to form many beams using multiple input ports in different directions from the aperture. To this end, a Rotman lens is useful in a variety of electronically steered applications. It provides a simple geometrical structure for beam switching and steering application by calculating the path difference from input ports to output ports. Planar microstrip lenses on a dielectric substrate reduce circuit size and manufacturing complexity through a simple etching process. In this research, a simple low-cost planar scanning array using a Rotman lens is designed using microstrip technology, as shown in Figure 1. A microstrip Rotman lens with 15 beam ports and 11 array ports is used as a feed for a multiple beam antennas to make the

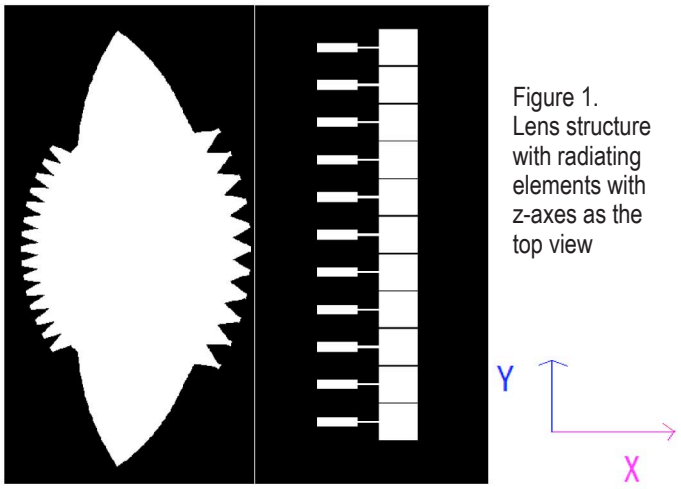

Figure 1. Lens structure with radiating elements with z-axes as the top view

scan angle of -45 degrees to +45 degrees (off axis beam scanning angle).

Theoretical Design Formulations:

Referring to Figure 2[1], the following design equations are used to select the initial design parameters for the lens. In order to calculate the values of w, which are the electrical lengths of the transmission lines required to connect the individual antenna elements to ensure that all paths that reach the z contour are in phase, equation $Aw^2+Bw+C=0$ is used. This equation gives the relationship between w and A, B, and C variables as follows [1]:

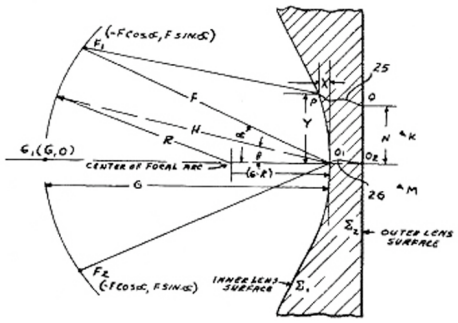

Figure 2. Rotman lens geometry

$$A_i = 1-\eta_i^2-\left(\frac{g-1}{g-a_0}\right)^2;\quad B_i = 2g\left(\frac{g-1}{g-a_0}\right)-\frac{(g-1)b_0^2\eta_i^2}{(g-a_0)^2}+2\eta_i^2-2g;$$

$$\text{And}\quad C_i = \frac{gb_0^2\eta_i^2}{g-a_0}-\frac{b_0^4\eta_i^4}{4(g-a_0)^2}-\eta_i^2,$$

Where g, n_i, a_0 b_0, represents normalized on axis focal point, normalized position of the array contour, cosine and sine function of the maximum angle of scanning respectively.

To find the lengths of the transmission lines between the array contour and the lens, we solve the design equation for w:

$$W_i = \frac{-B_i-\sqrt{B_i^2-4A_iC_i}}{2A_i}.$$

Substituting w values into the following equations [2] provide the corresponding coordinates for the location of various ports along the lens contour, y. (The following values have been converted to cm for placement into CAD design)

$$X_i = \frac{2W_i(1-g)-b_0^2\eta_i^2}{2(g-a_0)}F_\lambda\lambda_d;\quad \text{and}\quad Y_i = \eta_i(1-W_i)(F_\lambda\lambda_d),$$

The final theoretical scanning pattern as a result of these parameters is depicted in Figure 2. There are a total of fifteen scanning positions. The designed 3-dB beam widths is 6° that widens, as expected, as the beams are scanned off bore axis.

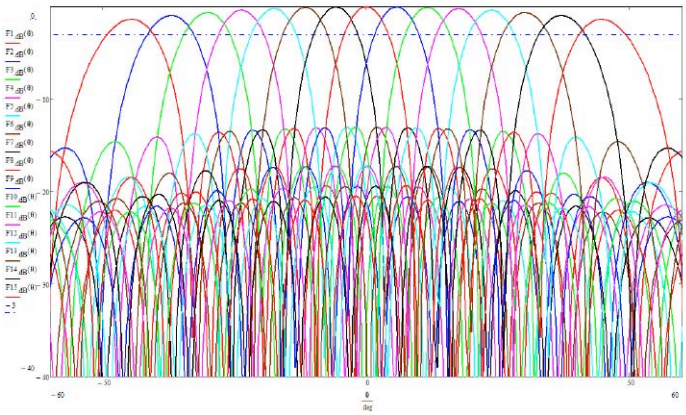

Figure 3. Beam patterns at various antenna ports

ANSOFT Simulations

During this phase, the theoretical design parameters were input to ANSOFT's Designer software to optimize the design parameters given a particular lamination board. Various lens structures were designed using AutoCAD to simulate and to obtain optimized results. Finally, optimized S parameters were obtained.

The beam patterns over the patch elements are obtained by feeding the S_{12} values to the input of the patch elements, spaced 0.5λ apart. Figures 3-4 below depict the patterns corresponding to two beam ports, located at zero degrees and at -45 degrees.

The gain and the efficiency of the array are calculated as [3].

$$\Omega_A = \frac{\int_0^{2\pi}\int_0^{\pi}|F(\theta,\phi)|\sin\theta d\theta}{|F(\theta,\phi)|^2};\quad D=\frac{4\pi}{\Omega_A};\quad G=\eta D=(1-\delta)D;\ \text{and}\ \delta=\text{Loss tangent}.$$

Using the equation above, the relative permittivity $\varepsilon_r \rightarrow 2.2$ and loss tangent $\rightarrow 0.009$, the max gain of the antenna array is calculated to be 15.095 dB, and the max gain from the simulation was recorded to be 15.055 dB.

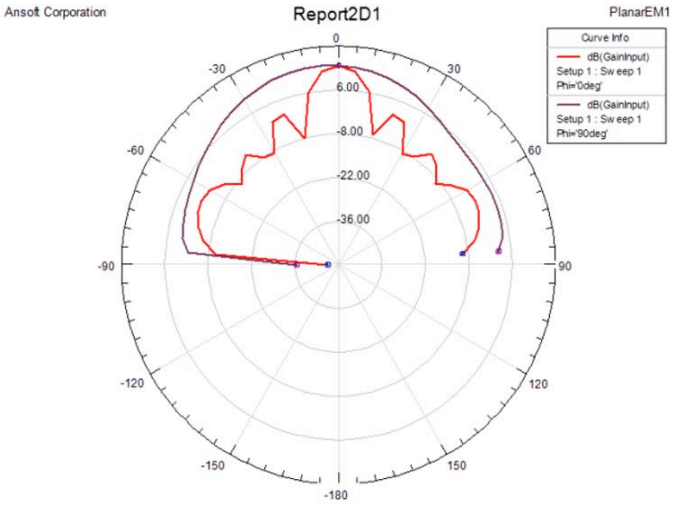

Figure 4(a). Far-field Polar power pattern corresponding to central port at zero degrees

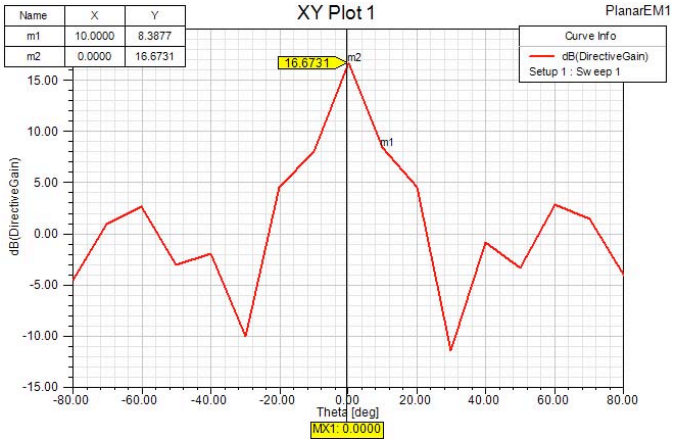

Figure 4(b). Far-field Linear power pattern corresponding to central port at zero degrees

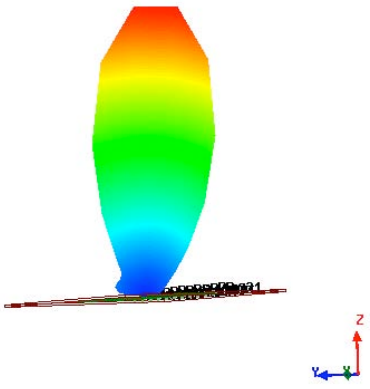

Figure 4 (c). 3-D beam pattern in Y-Z plane, corresponding to port at zero degrees

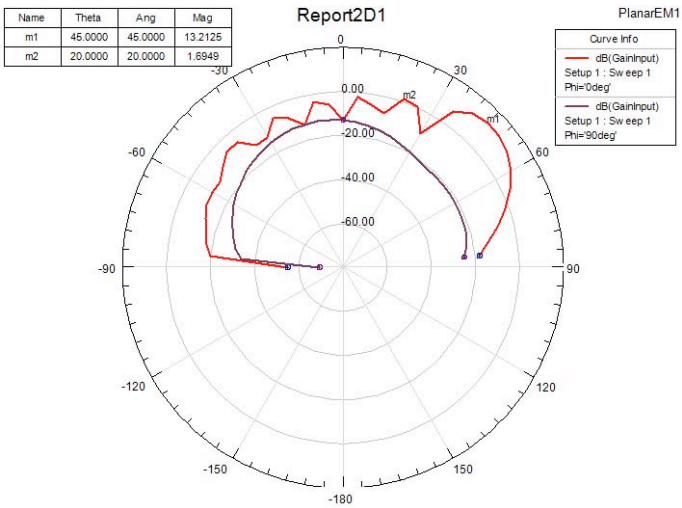

Figure 5(a). Far-field Polar power pattern corresponding to port at -45 degrees

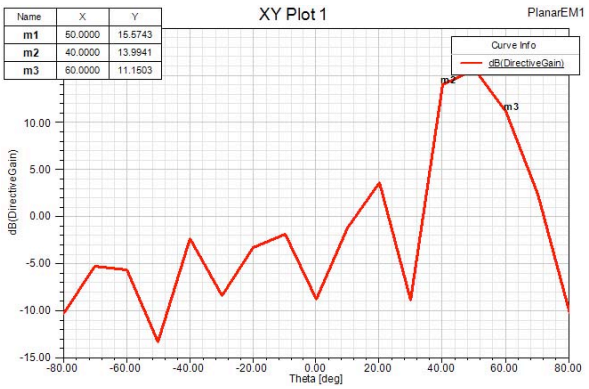

Figure 5(b). Far-field Linear power pattern corresponding to port at -45 degrees

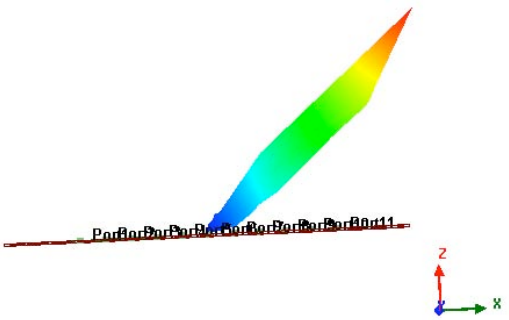

Figure 5(c). 3-D beam pattern in Y-Z plane corresponding to port at -45 degrees

The Insertion and Reflection losses as depicted in Table I and II are obtained. As expected, the ports located at +/- 45° suffer from the highest insertion loss.

Table I: Insertion loss corresponding to various beam ports

BEAM PORT (N)	INSERTION LOSS (DB)	BEAM PORT (N)	INSERTION LOSS (DB)	BEAM PORT (N)	INSERTION LOSS (DB)
1	3.758	6	3.118	11	3.0080
2	2.858	7	2.995	12	2.958
3	3.012	8	3.113	13	3.103
4	2.971	9	2.999	14	2.874
5	3.034	10	3.079	15	3.664

Table II: Reflection loss corresponding to various antenna ports

ANTENNA PORT (N)	REFLECTION LOSS (DB)	ANTENNA PORT (N)	REFLECTION LOSS (DB)	ANTENNA PORT (N)	REFLECTION LOSS (DB)
1	-4.856	5	-5.09	9	-5.07
2	-4.979	6	-5.08	10	-4.99
3	-5.07	7	-5.08	11	-4.861
4	-5.10	8	-5.10		

Table III: Theoretically calculated 3-dB beam widths, side lobe levels, and max beam positions

PARAMETERS	PORT1	PORT2	PORT3	PORT4	PORT5	PORT6	PORT7	PORT8
BEAM-WIDTH(DEG)	10	9	8	7	6.5	6.5	6	6
SIDE LOBE LEVEL(DB)	-15	-14.3	-13.9	-13.7	-13.5	-13.2	-13.1	-13.0
MAX BEAM POSITION (DEG)	-45	-37	-30	-23.5	-17.5	-11.5	-5.5	0

Table IV: Simulated 3-dB beam widths, side lobe levels, and max beam positions

PARAMETERS	PORT1	PORT2	PORT3	PORT4	PORT5	PORT6	PORT7	PORT8
BEAM-WIDTH(DEG)	10	9.2	8	7	6.5	6.5	6	6
SIDE LOBE LEVEL(DB)	-11	-13.2	-13	-13	-12.7	-12.8	-12.5	-13
MAX BEAM POSITION (DEG)	-50	-40	-32	-25	-19	-12	-7	0

Comparison Between Various Theoretical and Simulated Results:

The theoretical designed 3-dB beam widths and simulated 3-dB beam widths are shown in Tables III and IV. Also shown in these tables are the values for max side lobe levels and the max beam positions. Due to the symmetry of the lens structure only one side of the lens is depicted in Tables III and IV.

It may be observed that the theoretically designed 3-dB beam width is six degrees, and is only achieved at three central ports. It widens to 10 degrees as we scan off bore axis to either +/- 45 degrees. Simulated results related beam widths are almost identical to that of theoretically calculated.

Theoretical Sidelobe Levels (SLL) are around -13 dB corresponding to a rectangular input feeding arrangement; the simulation results are nearly identical to that of theoretical ones, deviating somewhat corresponding to ports at +/- 45 degrees.

There is, however, a large error in terms of positioning of max beams when compared with that of corresponding theoretical beam positions. This error gets as large as about five degrees when beams are scanned to +/- 45 degrees.

Change in Research Direction

Two of the parameters, namely 3-dB beam widths and maximum beam positioning angles at or close to intended scanning angles +/- 45 degrees will not be met; thereby, necessitating a rethink in our design. In our new approach, the lens is designed for +/- 26 degrees; this will then be combined at an angle to cover the entire +/- 45 degrees sector.

Significance

Most of the intended work for this project, as per the original proposal, has been completed on time. The results obtained through theoretical formulations and that of using ANSOFT's simulation software are in broad agreement. The first prototype that was developed did not yield desired results, necessitating a revised and updated design. This design is currently under fabrication and is likely to be ready in about two weeks. Thereafter, the testing and consolidation of experimental data/results is likely to take about four weeks. Additionally, this project has been extended for another year to fabricate and test a full-scale prototype. The main tasks to be accomplished during the second year of this project are: preparing a design for a switching network, identifying and acquiring these components; assembling and testing the final system in the anechoic chamber; and comparing the experimental results with that of simulations.

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[2] R. Jedlicka, "Microstrip Analysis and Synthesis," April 1995

[3] C. Balanis, "Antenna Theory Analysis and Design," 3rd edition, John Wiley & Sons, 2005

High-capacity, Cooperative Wireless Code-division Multiple-access (CDMA) Networks via Per-antenna Adaptive Modulation (PAAM) and Turbo Space-time Adaptive Interference Suppression

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Abstract

We have addressed two problems encountered in wireless communication systems. First, although Direct Sequence Spread Spectrum (DS-SS) methods are inherently capable of suppressing narrowband interference (NBI), as spectrum becomes more crowded, this processing gain become insufficient. We have developed an active NBI suppression scheme that explicitly suppresses multiple types of NBI signals, with different power levels. Second, the channel outage due to random wireless fading is a severe problem. Multiple antenna techniques are commonly proposed for combating fading. However, when having multiple antennas at the transmitters are not a realistic option, we have developed a cooperative communications protocol to improve the outage throughput of a DS-SS system using this concept of cooperative relaying.

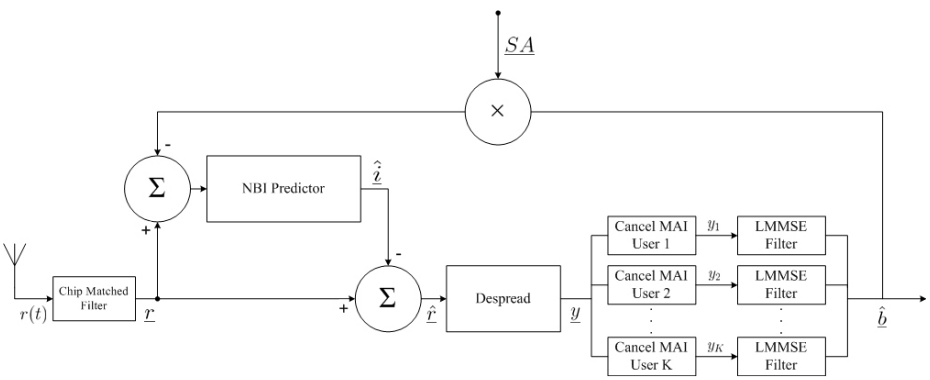
Accomplishments

During this project, we have developed a new receiver structure for a DS-SS system that can suppress both different types of narrow-band interference and the wideband multiple-access interference from other spread-spectrum users simultaneously. The proposed receiver employs a Kalman predictor to remove the NBI and a bank of linear Minimum-Mean-Squared-Error (MMSE) filters to suppress the wideband multiple-access interference. The receiver then makes use of the powerful iterative (turbo) processing concept to feedback the soft outputs of user symbols from one iteration to another, to cancel out the spread-spectrum user signals. A block diagram of the developed receiver is shown below.

So far, the implemented version of this receiver in MATLAB is capable of handling auto-regressive NBI processes and multiple spread-spectrum users. Currently, we are implementing the scheme to handle both auto-regressive and digital narrowband interferes. The receiver then would be able to handle a mix of different NBI sources as well as other wideband interferers at the same time. The analytical modeling of our work provides a unified framework for taking into account both types of narrowband interferers that may co-exist in the same frequency band of interest.

Cooperative communications have been proposed as an alternative to having multiple-transmit antennas, when physical constraints prevent one from being able to implement an antenna array with multiple elements. These schemes work by users relaying each other's signals. Such cooperative relaying can provide spatial diversity against channel fading. However, previously proposed cooperative communication schemes do not increase throughput in the high Signal-to-Noise Ratio (SNR) region although they improve the outage probability. This is because cooperative communication sacrifices throughput for reliability. In this project, we developed a new cooperative communications protocol for direct-sequence code-division-multiple-access (DS-CDMA) systems that increases the SNR range over which there is no significant throughput loss compared to direct transmission. This eliminates the necessity for switching between more than one scheme, which leads to higher system complexity.

The new cooperative communications protocol developed during this project has a high spectral efficiency (reaching unity asymptotically with the SNR and block size), at the cost of



extra spreading sequences. However, the spreading codes are allowed to be non-orthogonal, and we have analyzed the effect of that on the resulting cooperative diversity under both matched-filter-based as well as the linear MMSE (LMMSE)-based receivers. We have also derived both achievable and outage throughput under different cross correlations between user codes. From our simulation results (in MATLAB) it can be seen that the proposed new cooperative protocol improves the throughput and the outage throughput performance in high SNR at the expense of only a negligible loss in the low SNR region compared to the previously proposed reference schemes.

Significance

The work on cooperative communications protocols is expected to be continued by looking into improved algorithms as well as their performance limits. The PI expects to seek other funding to support this research in the near future.

Publications

A.V. Kariyapperuma and S.K. Jayaweera, "An Asymptotically Full Rate Cooperative Communications Scheme for DS-CDMA Systems with Non-orthogonal Codes," International Symposium on Information Theory and its Applications (ISITA2008), Auckland, New Zealand, December 2008. Accepted for publication.

Reduced-order Modeling of Shear Layers

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Abstract

Shear layers are often viewed as local "model flow" for other complex configurations. However, to accurately describe this simple flow, a system space in very high or even infinite dimensions is still required. The main objective of this project is to develop reduce-order models (ROM) for both temporally and spatially evolving shear layers. ROMs are able to describe most physics in much lower dimensions and reduce the computational complexity, and, more importantly, enable the direct usage of many dynamic systems and control theories. The general technique is under the framework of Proper Orthogonal Decomposition (POD) and Galerkin projection. However, a symmetry reduction concept from geometric mechanics will be introduced to modify the approach that more aggressive model reduction can be obtained.

Accomplishments

Free shear layers are often studied as model flow for its simplicity. The behavior of temporally or spatially developing shear layers has been, of course, studied widely for decades from theoretical, numerical, and experimental aspects. However, shear flows are still too complex to directly apply dynamic systems and control theories, which have been widely used to analyze and understand many simple mechanical systems. Though low-dimensional models have been proposed and have succeeded in some applications, they are mainly phenomenological. Our goal for this work is to develop low-dimensional models for shear layers from the direct projection of Navier-Stokes equations.

Unlike conventional POD/Galerkin projection, we introduced a scaling variable g to map the whole problem to a symmetry-reduced space and then obtain ROMs with much lower dimensions in the new space. The original Navier-Stokes equations used to describe shear layers are, therefore, reduced to an Ordinary Differential Equation (ODE) system with only three variables (or five variables for more complex cases). The results of using this approach to model temporally developing shear layers have been accepted for publication in the Journal of Fluid Mechanics.

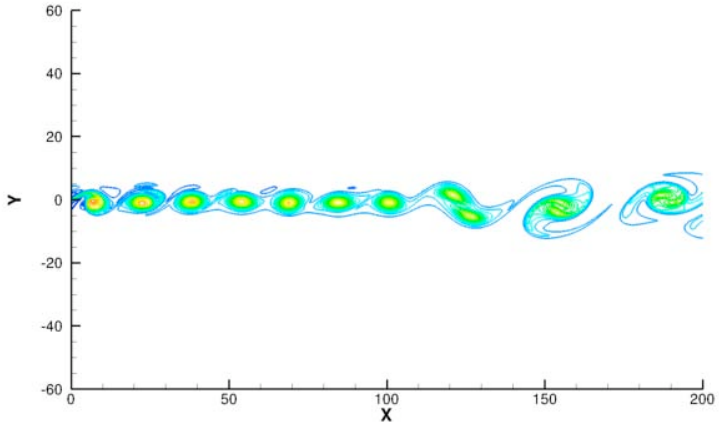

Figure 1. Schematic of a spatially developing free shear layer

Continuing the success in temporally developing shear layers, we also derived the dynamical equations for spatially developing shear layers (Figure 1). The main difficulty for spatial modeling is that the governing equations (e.g., Navier-Stokes equations) are not simply parabolic (or hyperbolic) in space. This embedded ellipticity prevents the system from being described by an ODE system marching in space. To solve this problem, we first parabolized the equations using boundary-layer assumption which can be justified for thin shear layers. The parabolic-downstream equations allow us to apply the same modified POD/Galerkin projection approach with a downstream scaling variable $g(x)$ to factor out viscous growth. The dynamical system for the mode coefficients $a = (a_{1,1}, a_{1,2})$ is

$$(B - C)\dot{a} = \left[H + \frac{1}{\mathrm{Re}} g^2 D + \frac{\dot{g}}{g} E\right] a$$

with well defined coefficients matrices. Together with the evolution equation for $g(x)$,

$$\dot{g} = \frac{\left(c_{01} a_{1,1} a_{1,1}^* + c_{02} a_{1,2} a_{1,2}^* + c_{03} a_{1,1} a_{1,2}^* + c_{04} a_{1,2} a_{1,1}^*\right) g + \frac{1}{\mathrm{Re}} d_0 g^3}{b_{01} + b_{02} a_{1,1} a_{1,1}^* + b_{03} a_{1,2} a_{1,2}^* + b_{04} a_{1,1} a_{1,2}^* + b_{05} a_{1,2} a_{1,1}^*},$$

the system in much lower dimensions is well defined. It is noticed that the scaling variable is dynamically computed and brings a great flexibility under different flow conditions.

During this project, the collaboration between the NMSU PI and Sandia collaborators has been strengthened in many ways: 1) monthly teleconference has been arranged and provided great outcome for ideas and future opportunities each time; 2) NMSU PI has given a seminar at Sandia, and two Sandia collaborators have given a joint seminar at NMSU. The seminars, together with other regular on-site visiting, provided the communication between NMSU and Sandia in a broader scope; 3) a conference paper will appear early next year for the work done together by the supported graduate student, NMSU faculty and Sandia collaborators.

The research and collaboration will be continued by the second year support from SURP.

Publications

M. Wei and C.W. Rowley, "Low-dimensional Models of a Temporally Evolving Free Shear Layer", *J. Fluid Mech.* (in press), 2008

B.R. Qawasmeh, M. Wei, M.B. Barone, and B.G. van Bloemen Waanders, "Low-dimensional Modeling for Spatial Developing Free Shear Layer," 47th AIAA Aerospace Sciences Meeting, AIAA paper 2009-363 (to appear), 2009

B.R. Qawasmeh and M. Wei, "Projection of Spatial Shear Layers in a Symmetry-reduced Space", 61st Annual Meeting of the APS Division of Fluid Dynamics, November 23-25, San Antonio, Texas, 2008

Control of the Structural Boundary Conditions using Piezoelectric Elements and Shunt Circuits

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Abstract

Advanced engineering structures incorporate boundary conditions that deviate from classical free, pinned or fixed cases. These conditions affect structural dynamic characteristics and need to be accounted for during structural testing. A modern approach for control of structural boundary conditions employs piezoelectric shunt circuits in which the mechanical strain, transformed by the piezoelectric material into the electrical voltage, is altered by the elements of the electrical circuit. This project is focused on development of theoretical and experimental foundations of the technology for control of structural boundary conditions. It is anticipated that availability of such a technology could improve accuracy of structural dynamic testing.

Accomplishments

In this project, the shunted piezoelectric technology for control of structural boundary was investigated. Investigations were carried out along three major directions: analytical modeling, numerical modeling, and experimental testing.

In the first stage of the project, an analytical approach for modeling piezoelectric elements with an additional shunt circuit was verified. The approach was further extended into representation of the model using an equivalent electrical circuit and incorporating additional complexities such as metallic caps. Comparison of the active element analytical model with experimental data shows reasonable match. Addition of the shunt circuit to the piezoelectric element yields similar changes in calculated and measured impedance responses as indicated in Figure 1.

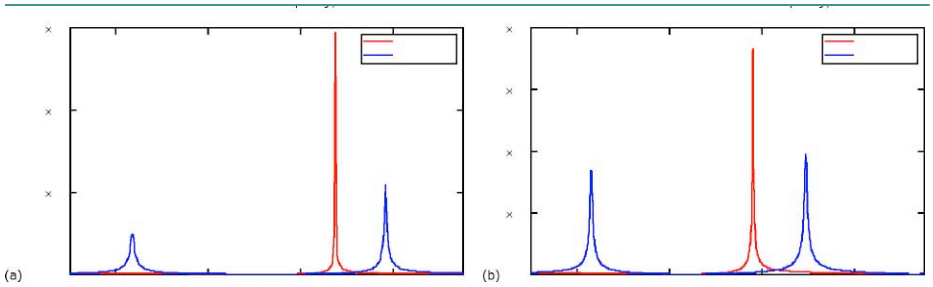

Figure 1. Theoretical (a) and experimental (b) real impedances of EDO EC-64 connected in parallel with inductor L = 10.44 mH

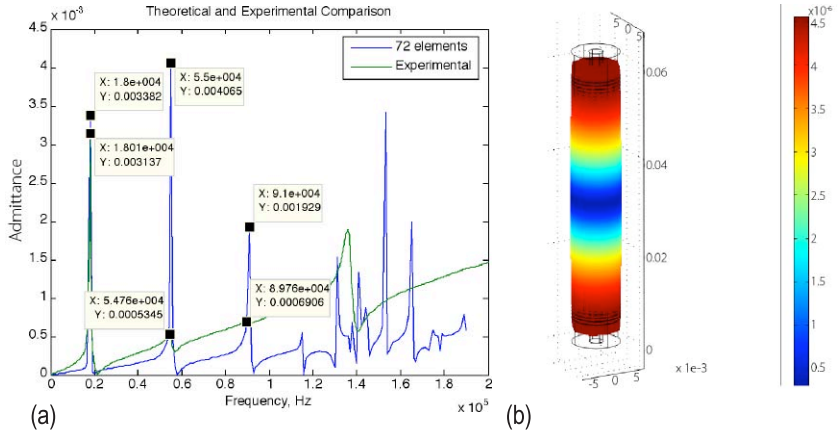

Figure 2 (a). Comparison of the 72 elements numerical model with the experimentally measured admittance; (b) vibration mode of the stack at 18 kHz

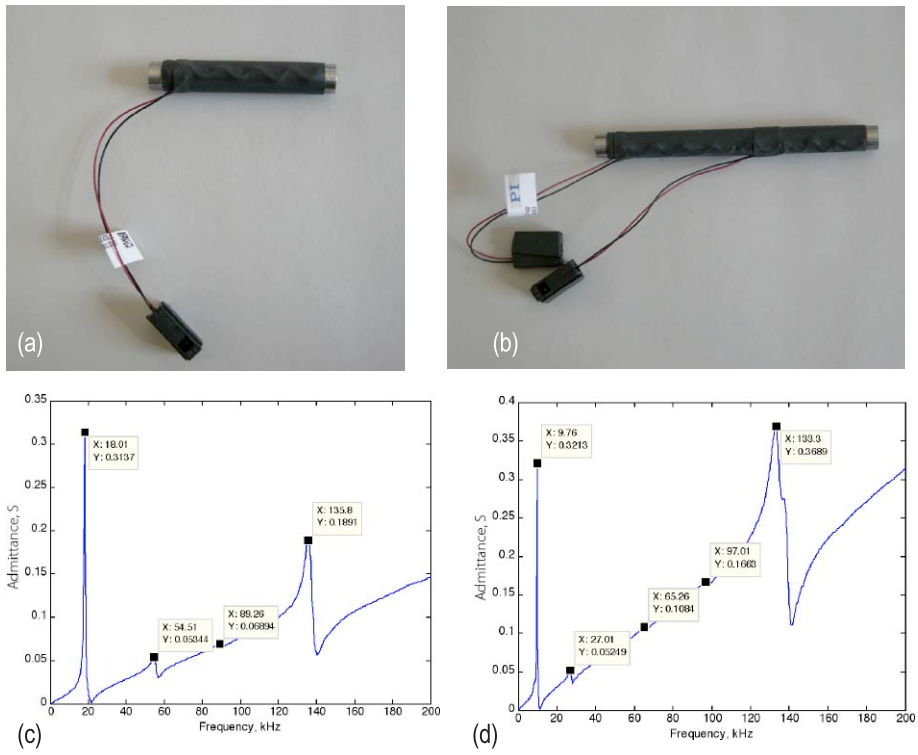

Figure 3. Short (a) and long (b) piezoelectric stacks; (c) experimentally measured admittance of short piezoelectric stack; (d) experimentally measured admittance of long piezoelectric stack

To account for complex geometries of the structure and the piezoelectric element, numerical finite element models were considered. The numerical approach was tested on a model for a single piezoelectric element. The finite element model allowed for precise calculation of admittance of the piezoelectric and provided visualization of vibration mode-shapes. The numerical approach was utilized to model a piezoelectric stack provided by Sandia. It was found that a model with 72 piezoelectric elements (rather that 104 as in actual stack) yielded a very good description of stack's dynamics (Figure 2).

Experimental testing in this project was conducted using impedance analysis. Implementation of impedance testing provided opportunities for measuring characteristics of active elements such as short and long stacks supplied by Sandia (Figure 3). An improved impedance measurement setup was utilized for observing nonlinear behavior of piezoelectric material.

An analytical model based on equivalent electrical circuit analysis was developed for a simple structure (aluminum bar) with shunted piezoelectric boundary condition. The model accounts for longitudinal vibrations of both structure and piezoelectric element. It was found that, when a piezoelectric was connected to one side of the aluminum bar, the model yielded a response closely resembling the clamped-free boundary conditions. Addition of the electrical shunt circuit yielded relatively small changes of natural frequencies (several Hz). Experimental testing of the structural configuration described by the model resulted in even smaller difference between shunted and non-shunted (open circuit) cases illustrated in Figure 4. An order of magnitude difference between theoretical and experimental values is not surprising because of limited

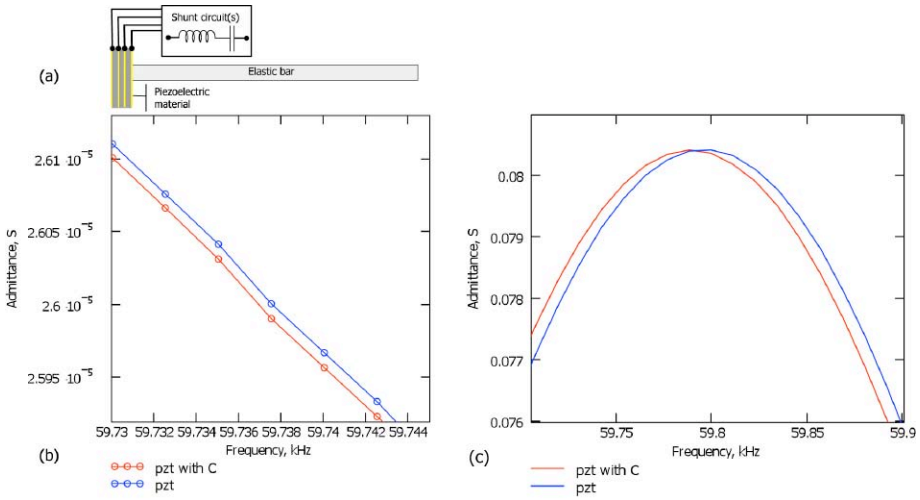

Figure 4(a). Design of the boundary condition control systems for longitudinal vibrations; (b) experimental data showing changes in frequency due to additional shunt circuit (58 μF); (c) theoretical responses indicating a frequency shift

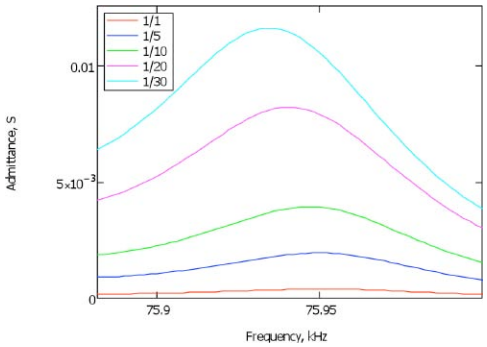

Figure 5. Admittance amplitude vs. frequency at increasing excitation levels. Frequency change indicates nonlinear behavior.

accuracy of the analytical, deviation of material characteristics, and relatively small capacitance used as in the shunt circuit. We conclude that although, in principle, piezoelectric-shunted circuits can be used to alter structural boundary conditions, changes of natural frequency provided by this approach are relatively small.

An additional dimension of this project was experimental study of the nonlinear response of the piezoelectric active element. Frequency deviation (6.5 Hz) due to nonlinearity was observed for the excitation voltage of 14 Volts (Figure 5). This deviation is comparable with frequency changes exerted by the shunt circuit. For this reason, accounting for nonlinear response is recommended when piezoelectric shunts are used for the boundary condition control.

Significance

Research efforts in this project were focused on experimental and theoretical support of Sandia's original and innovative idea on control of structural boundary conditions with piezoelectric elements and shunt circuit. Our research team contributed to analytical modeling, numerical simulation and experimental aspects of this new technology. For example, a system model that accounts for longitudinal resonances of piezoelectric active element was suggested and experimentally validated.

Developments in this project were carried out in accordance with the proposed plan. However, as the project progressed, two items were additionally considered due to their importance in practical applications. During development of the analytical model for boundary conditions control, it became apparent that numerical (finite element) simulation would be a desirable complement to the analytical model. Numerical simulations were conducted for piezoelectric elements of simple and complex (stack) geometries. In the latter case, it was found that a reduced model (72 piezoelectric elements versus 104 in original stack) yielded an accurate description of stack's dynamics.

In addition, Sandia's research indicated that nonlinearity of the piezoelectric device may noticeable affect in structural boundary control. Therefore, additional efforts in understanding nonlinear phenomena in piezoelectric material were carried out. An experimental setup was developed for testing nonlinear behavior of piezoelectric material and pilot tests were conducted.

This project had beneficial impact on on-going research and student training. The highlights are as follows:

1. One graduate student was funded for one year and results of the project will form a core of his thesis.
2. New Mexico Tech has developed capabilities to characterize piezoelectric sensors and actuators, which provides independent means of characterizing active materials.
3. New Mexico Tech developed structural dynamic testing capabilities for graduate and undergraduate education.
4. This project provided important impedance modeling and measurement skills that lead to better understanding of test procedures

and material performance. Improved understanding of electro-mechanical impedance principles allowed for generation of new ideas in the neighboring fields such as monitoring of structural health. Funding for these ideas is anticipated from DHS and DOD.

Publications

D. Kitts, A. Zagrai, T.S. Edwards, "Smart Materials for Electro-Mechanical Control of Structural Boundary Conditions," the 19th Annual Rio Grande Symposium on Advanced Materials, 9 October 2007, The University of New Mexico, Albuquerque, NM.

D. Kitts, A. Zagrai, T.S. Edwards, A. Zagrai, D. Kitts, W. Kruse, "Control of the Structural Boundary Conditions using Piezoelectric Elements and Shunt Circuits," New Mexico Tech Report # SURP-NMT-2007/2008-LISS-1. This is a detailed report on the project (57 pages 55 figures, 3 tables) submitted to Sandia collaborator. Available upon request.

SURP RESEARCH PROJECTS — Materials and Process Sciences

Quantum Dots for Melanoma Tumor Imaging

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Hongyou Fan (Org. 1815)
Sandia Principal Investigator

Abstract

Malignant melanoma has become a significant public health problem especially in the U. S. The development of effective new technologies for early detection and treatment of the disease becomes crucial. With Sandia's strong interest and capabilities in the areas of advanced materials and biosensing, the goal of the collaborative research program is to develop clinically useful diagnostic and imaging agents for detection, and tagging for the purpose of localization, staging, tissue biopsy, and fluorescence-directed surgical removal of melanoma tumors.

Accomplishments

As proposed, we planned to design and synthesize the potent and selective a-MSH peptides MT-I and MT-II (Specific Aim 1). We have synthesized MT-II. Meanwhile, we have synthesized the quantum dots (QDs) and immobilized on the surface of the QDs. We have characterized the properties of the peptide-conjugate QDs. Unfortunately, the nanoparticles are prone to aggregation in aqueous solution and thus cause significant toxicity (Figure 1). Therefore, we have decided to change the direction of the project and work on developing a highly sensitive and sensitive fluorescent reagent for the detection of highly toxic and pollutant thiophenols and explosive peroxides. Recently, we have developed fluorescence sensors for the detection of explosive peroxides and significant progress has been made.

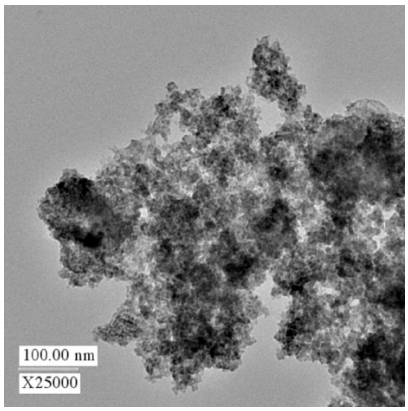

Figure 1. TEM image of MT-II conjugate immobilized QDs.

One of my long-standing research interests is to develop new materials for biological applications such as disease diagnosis, molecular imaging, and drug delivery. As a synthetic organic chemist with extensive experience in biomedical research areas, the PI is in a unique position for interdisciplinary research and collaboration. The PI's research team can design and synthesize any compounds with desired properties. On the other hand, Dr. Fan and his research team have extensive experience and expertise in the development of new materials. For example, Dr. Fan and his post-doc, Dr. Chen, have made several meso-porpous nanoparticles and magnetic nanoparticles. We also collaborate on the development of new fluorescent imaging probes for the detection of important chemicals. Recently, we have developed a highly sensitive and sensitive fluorescent reagent for the detection of highly toxic and pollutant thiophenols. To our knowledge, this is the first example of a highly selective chemical probe for thoiphenols over thioalcohols. The probe will have a great potential for practical application as a useful reagent for the detection of highly toxic chemicals.

Significance

The development of sensitive and selective imaging probes for detection of diseases and toxic and explosive substances is of considerable biological, scientific and life-saving significance. This application proposes to design and develop QDs-based imaging technology for the detection of malignant melanomas. According to our plan, we have made melanoma tumor cell specific MT-II conjugate quantum dots. Unfortunately, the nanoparticles are prone to aggregation in aqueous solution and thus cause significant toxicity. Therefore, we terminated the project.

The development of highly sensitive and selective sensing technologies for the detection of highly explosive peroxides is of considerable scientific and economic importance. An increasing number of incidents that involved the use of these explosive chemicals by terrorism groups have created a significant threat to the security, stability and economy of our society.

One reason peroxides have become one of the major chemicals for bomb production by terrorist groups is that these substances are readily accessed since they are commercially available or easily made in a straightforward manner from readily available precursor chemicals. The second reason is that these odorless chemicals can easily be concealed for entry into airplanes, trains and other public transportation means because sniffer dogs cannot detect them. Furthermore, peroxides cannot be detected by conventional explosive detection devices which, like those used at airports, rely typically on the presence of nitro compounds or metals for detection. Accordingly, the detection of odorless peroxides represents a formidable challenge. Recently, we have developed a highly sensitive and selective fluorescence probe for the direct and rapid detection of peracetic acid and benzoyl peroxide that does not require the use of complicated procedures and expensive facilities (Figure 2). This significant finding has been submitted for publication.

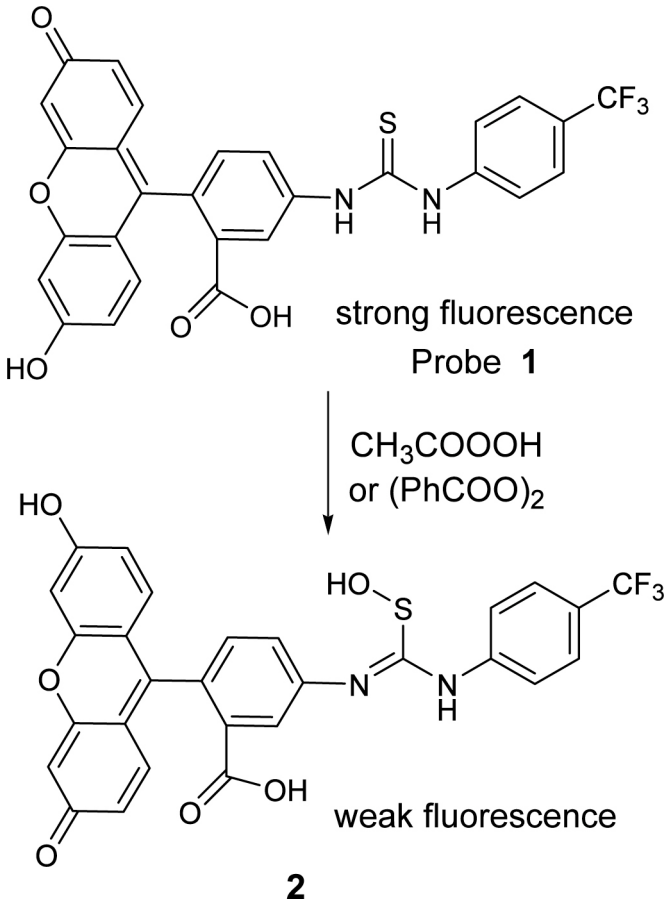

Figure 2. Fluorescent probe peracetic acids and benzoyl peroxides

Publications

W. Jiang, Q.-Q. Fu, H.-Y. Fan, J. Ho, and W. Wang, "A Highly Selective Fluorescent Probe for Facile Detection of Thiophenols," *Angew. Chem. Int. Ed.*, 46, 8445-8448, 2007

Q.-Q Fu, W. Jiang, H.-Y Fan, and W. Wang, "Highly Sensitive and Selective Fluorescence Sensors for Facile Detection of Peracetic Acid and Benzoyl Peroxide," Submitted to *Angew. Chem. Int. Ed.*

Conference Presentation

W. Jiang, Q.-Q. Fu, H.-Y Fan, J. Ho, and W. Wang, "A Highly Selective Fluorescent Probe for Facile Detection of Thiophenols," The 63rd Southwest Regional American Chemical Society Meeting, Lubbock, Texas, November 4-7, 2007 (both poster and oral presentation)

Improvement of MEMS Performance by Structural Vibrations

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John P. Sullivan (Org. 1132)
Sandia Principal Investigator

Abstract
Sticking contact (adhesion) between moving components in Micro-Electro-Mechanical Systems (MEMS) is a major problem which limits reliability. Sticking contact, referred to as "stiction failure," is fatal to the component; stiction prevents the individual component from operating properly and, hence, jeopardizes the reliability of the overall device. Currently, there are no commercially available MEMS or Nano-Electro-Mechanical Systems (NEMS) with contacting/sliding parts due to the reliability issue caused by adhesion failures. To enable their commercial introduction, practical techniques for the prevention of stiction and repair of failed devices under normal service conditions are required. The proposed methodology is a viable approach, enabling commercialization.

Accomplishments
An experimental setup now exists that can determine the different characterization parameters needed to model the repair of stiction-failed MEMS using structural vibrations. The setup is capable of determining the fundamental modes of the system, the elastic modulus of the material, and the damping of the system at pressures ranging from atmosphere to tens of mTorr. The setup showed that the theoretical values for these parameters match very well with the experimental values.

Once the characterization parameters are known, they can be used in the model to more accurately predict where initiation of debonding will occur for that specific system. By knowing where initiation of debonding will occur, it will be easier to predict the parameters that could ultimately repair the MEMS device.

Modeling work has been undertaken that predicted instability regions appearing around the natural frequencies of the system, and the size of the instability region increases proportionally with the applied voltage. The experimental data also showed that voltages below 5V could create instability in the system, and 5V is easily attainable for most systems in which MEMS are used. This means it would be feasible to repair stiction-failed MEMS with structural vibrations in-service.

Not only were instabilities observed, but the application of structural vibrations also repaired numerous beams. At one point, repair of an s-shaped stiction-failed beam occurred at a single frequency near the third mode at a voltage of less than 5V.

An additional apparatus has recently been completed that allows for the measurement of interfacial shear energies for failures in Modes I, II, and III. No measurements have been made to date. Completion of this goal is the end of the second quarter in Year 2 of this funding. Summarizing the accomplishments to date:

- 2 conference papers have been published [1, 2]
- 2 journal papers are in progress [3,4]
- 1 MS student has passed his defense with distinction[1], an additional student has begun work on this project and will graduate in summer 2009
- Interactions with John Sullivan, Sandia Principal Investigator
  - Center for Integrated Nanotechnologies (CINT)
    - Use of LDV has led to observance of Mathieu-type behavior
    - CINT User proposal accepted – U2008A013
  - John Sullivan, Sandia PI, served on the defense committee of the MS student that graduated with distinction

Significance
Two additional grants were applied for and awarded based on this research. The National Science Foundation (NSF) gave the first follow-on award. This work was submitted twice to the Dynamical Systems Program of the Division of Civil, Mechanical, and Manufacturing Innovation. The title of the proposal was "Improvement of MEMS Performance by Structural Vibrations: Theory and Practical Implementations."

The proposal included results generated by the SURP Year 1 work. These results were important to the success of this proposal. Work included in this proposal is an extension of what was proposed in the present SURP work. Besides a broader experimental effort, a theoretical effort was included. The theoretical work will be done with Kevin Murphy in the Mechanical Engineering Department at the University of Connecticut.

Both reviews of the proposal were extremely positive. The first review of the proposal did not receive funding due to budget constraints; the second review was funded (**CMMI-0826580** / http://www.nsf.gov/awardsearch/showAward.do?AwardNumber=0826580). The principal investigator for the NSF proposal was Zayd Leseman. The

[1]About 1 student per year receives this distinction in the Mechanical Engineering Department at UNM

proposal was funded at a level of $80k/year for three years (Aug 2008 – Aug 2011).

The second award granted was the second-year funding for this same proposal from SURP for continuation through the year 2 goals. Year 1 goals were met and all indicators show that year 2 goals will be successfully completed as well.

References

[1] D.F. Goettler, A. Savkar, K. Murphy, and Z.C. Leseman, "Repair of Stiction-Failed MEMS Using Structural Vibrations," in *ASME Micro-Electro-Mechanical Systems (MEMS) IMECE2007*, Seattle, WA, p. 7, 2007

[2] D.F. Goettler, M.R. Kashamolla, and Z.C. Leseman, "Repair of Stiction-Failed MEMS Using Structural Vibrations," in *ASEE Gulf-Southwest Annual Conference*, Albuquerque, NM, p. 12, 2008

[3] D.F. Goettler, Z.C. Leseman, A. Savkar, K.D. Murphy, and J.P. Sullivan, "Stiction Failure of MEMS/NEMS and Their Repair," work in progress.

[4] D.F. Goettler, Z.C. Leseman, and J.P. Sullivan, "Experimental Measurements of the Structural and Squeeze Films Damping Parameters in MEMS," work in progress.

SURP RESEARCH PROJECTS – New Initiative – Bio

Development of a Cell-based "Smart" Microfluidic Sensor

Heather Canavan
University of New Mexico

Ron Manginell (Org. 1744)
Sandia Principal Investigator

Abstract

This proposal describes the development of a cell-based sensor utilizing the surface modification with poly(N-isopropyl acrylamide) (pNIPAM) derivatized with a benzo-crown ether (BCE) moiety. The unique cell-release behavior of pNIPAM-BCE, combined with the ease of manufacture of microfluidic channels and plasma polymerizations, will allow the development of regenerable, continuous flow-through sensor/actuators for the rapid detection of host/pathogen interactions—the subject of Sandia's Microscale Immune Study Laboratory (MISL) Grand Challenge. The proposed research unites the unique capabilities of the PI at UNM (the use of thermoresponsive polymers for the non-destructive harvest of cells) with those of the co-investigators at SNL (fabrication of microfluidic arrays).

Figure 1. Photographs illustrating the rf plasma reactor. At left, silicon chips are loaded into the reactor atop a glass slide. At right, the plasma reactor during operation.

Accomplishments

Synthesis and characterization of pNIPAM substrates via plasma polymerization. Many methods have been reported to graft pNIPAM on surfaces. Previously, we demonstrated that plasma polymerization of pNIPAM (ppNIPAM) affords a one-step, solvent-free, vapor-phase method for the deposition of films that are sterile and pinhole-free, regardless of the surface chemistry or topography of the underlying substrate. In Year 1 of this proposal, the rf plasma reactor was fabricated at UNM (see Figure 1), based on a similar plasma chamber previously used by the PI. Briefly, the apparatus consists of a tubular glass reactor capable of operating in both pulsed and continuous wave mode, base pressure in the low 10^{-3} Torr range, and adjustable applied rf powers from 1-120W. We have modified the design of this reactor to include multiple monomer inlet ports, thereby making it enabling the deposition of mixed copolymers such as pNIPAM-BCE.

Due to the inherently energetic conditions of the plasma, it is extremely important to characterize the impact that key parameters (e.g., maximum rf wattage, pressure during deposition, location/position of the samples in the chamber) have on the resulting films. Therefore, the priority of Year 2 of the proposal was to characterize the ppNIPAM films using surface characterization tools. Using X-ray photoelectron spectrometry (XPS), the surface chemistries of ppNIPAM films deposited using this reactor were

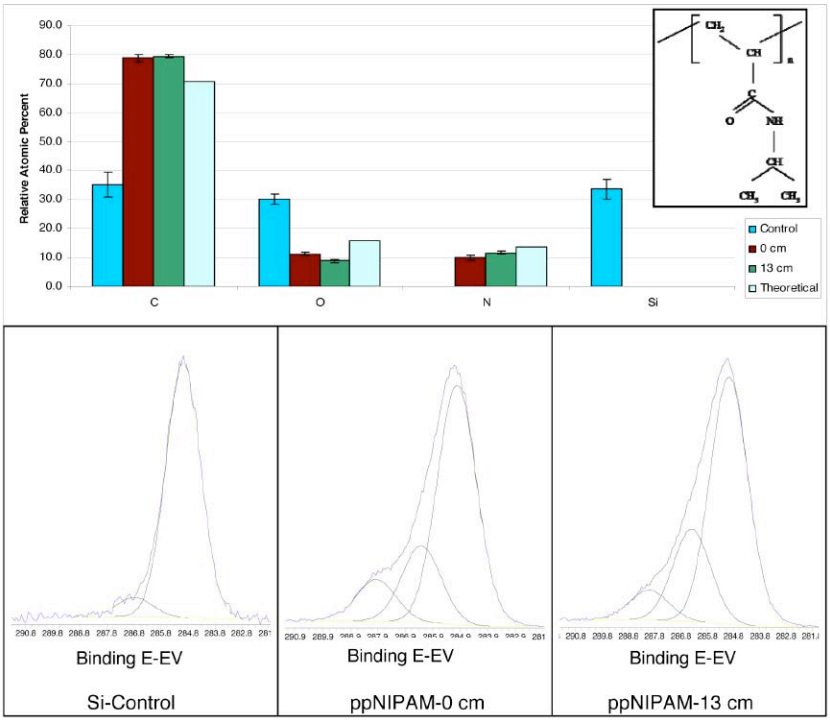

Figure 2. Surface composition of ppNIPAM surfaces by XPS (top). High res C1s spectra (bottom) of Si control (left), ppNIPAM upstream (mid), and ppNIPAM downstream (right).

evaluated (see Figure 2). In addition, time-of-flight secondary ion mass spectrometry (ToF-SIMS), contact angle measurements, and interferometry were used to optimize the surface chemistry, thickness, and thermoresponsive behavior of the films.

Cell attachment and detachment from ppNIPAM substrates. Subsequent to the demonstration of our ability to reproducibly generate thermoresponsive films, the cell-releasing properties of the ppNIPAM films were evaluated using the new mammalian cell culture facilities at UNM constructed in the lab of the PI. In this work, we tested the response of a variety of cell types, including yeast (*Saccharomyces cerevisiae*), bacteria (*Halomonas marina*), and mammalian cells (bovine aortic endothelial cells, BAECs). Briefly, ppNIPAM surfaces fabricated using the procedure described above were cultured to maturity at 37°C (i.e., > LCST {lower critical solution temperature} of pNIPAM). To test cell release, the culture media was

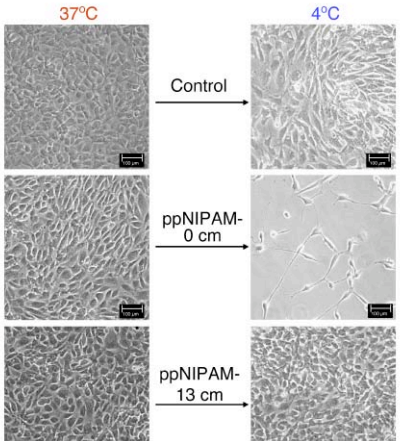

Figure 3. BAECs were cultured on TCPS control and ppNIPAM substrates. Cell adhesion (left) and detachment (right) was observed on control (top), ppNIPAM upstream (center), and ppNIPAM downstream (bottom).

removed and replaced with media below the LCST of the polymer (see Figure 3). The surfaces were observed using phase contrast microscopy and recorded using a digital camera such that the relative amount of bacteria adhered at each condition could be directly determined. Another priority for Year 2 was the optimization of the type of solution (e.g., serum-free media, media with serum, PBS, etc.) as well as the temperature at which the media should be used (i.e., below the LCST @ 25°C, or far below the LCST @ 4°C). As demonstrated in Figure 3, the ppNIPAM films generated using this reactor demonstrate the expected cell releasing properties. The results from this work were presented in numerous presentations, as well as a publication.

Publications

J.A. Reed, A.E. Lucero, M. Cooperstein, and H.E. Canavan, "The Effects of Cell Culture Parameters on Cell Release Kinetics from pNIPAM," *Journal of Applied Biomaterials & Biomechanics*, 6 (2), 81-88, 2008

Presentations

H.E. Canavan, "Plasma Polymerization of Thermoresponsive Poly(N-isopropyl acrylamide) for the Release of Multiple Cell Types," presented at the American Institute of Chemical Engineers Annual Meeting, Philadelphia, PA, November 16-21, 2008

A.E. Lucero and H.E. Canavan, "Optimizing an RF Plasma Reactor for Biocompatible 'Smart' Surfaces," presented at the American Institute of Chemical Engineers Annual Meeting, Philadelphia, PA, November 16-21, 2008

J.E. Fulghum, K. Artyushkova, A.E. Lucero, and H.E. Canavan, "Use of Multivariate Analysis Techniques to Predict Cellular Response to Plasma Polymerized pNIPAM," presented at the 54th International Symposium of the American Vacuum Society, Boston, MA, October 19-24, 2008

H.E. Canavan, "Use of 'Smart' Materials and Cell Sheet Engineering to Characterize Buried Biological Interfaces: Scientific and Engineering Applications," invited presentation to the Harvard University Department

of Engineering and Applied Sciences Summer Symposium, August 5, 2008

H.E. Canavan, S.L. Candelaria, J.A. Reed, A.E. Lucero, K.N. Wilde, X.P. Liu, and K.M. Gallagher-Gonzales, "Scientific and Bioengineering Applications of a Plasma Polymerized Thermoresponsive Surface," presented at the 3M Corporation Untenured Faculty Award Winners' Meeting, June 19-20, 2008

H.E. Canavan, S.L. Candelaria, J.A. Reed, A.E. Lucero, K.N. Wilde, R. Joe, P. Tapia, and M. Werner-Washburne, "Use of a Thermoresponsive Substrate to Separate Cell Populations," presented at the 8th World Biomaterial Congress, Amsterdam, the Netherlands, May 28 – June 1, 2008

A.E. Lucero and H.E. Canavan, "Optimizing Thermoresponsive pNIPAM Films using an RF Plasma Reactor," presented at the AAAS/ SWARM Symposium, Albuquerque, NM, April 11, 2008, honorable mention for best student poster

Hyperspectral Imaging, Multivariate Curve Resolution Analysis and Multi-color Single-particle Quantum Dot Tracking: Elucidating Membrane Protein Dynamics in Living Cells

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University of New Mexico

David Haaland (Org. 8632)
Sandia Principal Investigator

Abstract
The goal of this collaboration is to characterize quantum dots (QDs) for multiplex imaging using the hyperspectral microscope (HSM) and multivariate curve resolution (MCR) analysis developed at Sandia. The techniques developed here will be useful for the study of many different membrane protein dynamics in *living cells*. In addition, advancing the use of QDs for multiplexing is important to many fields, such as diagnostics and high-throughput screening.

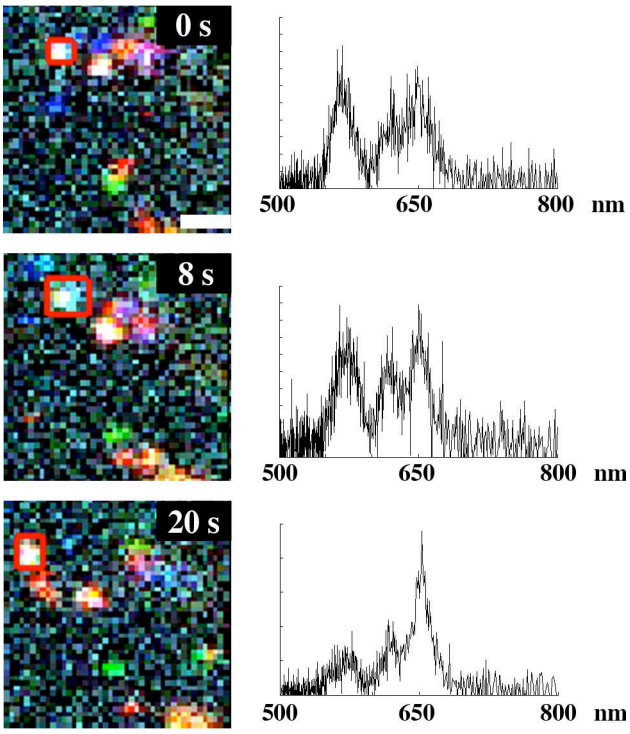

Figure 1. Hyperspectral images of QD-IgE-Fc_RI diffusion. After addition of crosslinker, stable receptor clusters are formed. Spectra of the cluster in the red circle show that three QDs (585, 625, and 655nm peaks) are present and remain together for 20s.

Accomplishments
We had previously generated a QD-tagged IgE that is capable of binding FcεRI and retains physiological activity. We have shown that it is possible to simultaneously image up to six spectrally distinct QDs on living cells. In addition, we can track the QD-labeled receptors at the single molecule level. These experiments allow us to determine if multiple QD-labeled receptors are in a cluster and the stability of those clusters. For example, in the resting state, QD-IgE-FcεRI can be seen to transiently co-localize. After activation by addition of crosslinking antigen, multiple QD-IgE-FcεRI complexes remain co-localized for long times. These experiments have also revealed that small clusters of crosslinked receptors (dimers or trimers) are still mobile (Figure 1), indicating that immobilization is not required for signal initiation.

The exploration of MCR analysis techniques applied to single QDs has revealed the possibility that there is enough heterogeneity between QDs of the same class for unique identification. The implication is that we may not be limited to separating QDs by distinct color classes but can distinguish every individual QD as unique, opening the possibility for a dramatic increase in the multiplexing capability of QDs. Statistical analyses on the time-resolved emission spectra of individual QDs bound to glass showed that the spectral peak and width of each QD is constant over time. Rigorous analysis of this

data is ongoing, in order to develop techniques for separating QDs of the same class within an image.

Significance

The analysis of temporally resolved hyperspectral images of multi-QD-labeled IgE proteins on cells has led to an important discovery. Examination of the raw spectral data clearly showed image pixels with spectra for each of five classes of QDs added to the cell membrane (565, 585, 625, 655, and 705 nm). However, our multivariate curve resolution (MCR) analysis of the hyperspectral image found only two classes of QDs. This finding led to the discovery that the loss of information was due to the principal component analysis (PCA) that is applied before MCR analyses are performed. PCA compression is a universal practice in the MCR analysis of hyperspectral images. However, in the images of the QDs, PCA compression loses information about the QDs due to correlated read noise in the spectral image. Since the PCA factors retained are in order of highest to lowest variance, PCA truncation causes QD information to be lost.

After this discovery, we found that the correlated noise was randomly distributed throughout the spectral images. Therefore, simple spatial averaging of spatial pixels results in a reduction of the level of correlated noise without appreciably affecting the QD signals. By first spatially compressing the spectral image followed by PCA and MCR, we were able to recover the pure spectra of all five QDs. Once these pure QD spectra were obtained, we could project the pure spectra onto the spectra at the original spatial resolution to obtain concentration maps at the original diffraction-limited spatial resolution.

As a result of this successful collaboration, we have submitted an NIH R21 application to build a hyperspectral microscope at UNM. This application has received a favorable score. The grant is led by Keith Lidke (UNM Physics), with Diane Lidke (UNM Pathology) and Michael Sinclair (Sandia) as co-investigators.

This work has resulted in an oral presentation by Lidke at the SPIE Photonics West Meeting in January 2007, as well as a publication in the *Proceedings of SPIE*. SURP support for the development of the QD-IgE probe lead to a recent Nature Cell Biology paper. Two further manuscripts that directly use hyperspectral data are in preparation and an abstract has been submitted for presentation at the Biophysical Society Meeting in February 2009.

Publications

D.S. Lidke, N.L. Andrews, J.R. Pfeiffer, H.D.T. Jones, M.B. Sinclair, D.M. Haaland, A.R. Burns, B.S. Wilson, J.M. Oliver and K.A. Lidke, "Exploring Membrane Protein Dynamics by Multicolor Single Quantum Dot Imaging using Wide Field, TIRF, and Hyperspectral Microscopy," *Proceedings of SPIE*, 6448:6448Y1-8, 2007

N.L. Andrews, K.A. Lidke, J.R. Pfeiffer, A.R. Burns, B.S. Wilson, J.M. Oliver and D.S. Lidke, "Actin Restricts Fc_RI Diffusion and Facilitates Antigen Induced Immobilization," *Nature Cell Biology*, 10:955-963, 2008

Two other manuscripts are in preparation.

Application of Molecular Techniques to the Study of Microbial Biofilms

Cristina Takacs-Vesbach
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Susan Altman (Org. 6316)
Sandia Principal Investigator

Abstract

Aquatic microbial biofilms are ubiquitous in nature and are responsible for considerable environmental problems including biofouling, microbial mediated corrosion, and the persistence of pathogens in drinking water distribution systems. The development of effective, sensitive, yet rapid monitoring tools is critical for understanding biofilm composition, growth, and physiological response to our efforts to control them. We developed a rapid, sensitive assay to monitor the growth and physiological state of microbial biofilms that has all of the strengths of the commonly used techniques, such as plate counts, but is more specific and can distinguish between live and dead cells.

Accomplishments

We developed a real time Polymerase Chain Reaction (qPCR) assay for microbial RNA and DNA that uses a combination of various primers and probes to study the development of single species and drinking water (complex) biofilms. We evaluated whether this method could be used to monitor the entrainment and persistence of potential pathogens in these systems. Additionally, we determined whether the method was sensitive enough to detect the effects of chlorination and regrowth and compared our results to simultaneous monitoring by plating. We found that the qPCR assay was

as sensitive as plating, but revealed a different physiological response to chlorination than detected by plating. After chlorination, plate counts indicate that biofilm biomass is decreased. However, our DNA qPCR indicates that biomass is unchanged in the biofilm, but the RNA qPCR revealed that the biofilm cells are more active, presumably due to cellular stress from chlorination. Thus, the decreased plate counts are an indication of the biofilm entering a viable, but not culturable state during chlorination treatment, which is consistent with biofilm recovery as evidenced by an increase in plate counts once chlorination stress is removed.

Publications

E. Crossey, C.D. Takacs-Vesbach, G. Ryan, and S. Altman, "Rapid Quantification of Microbial Biofilms and Assessment of Physiological State Using a Real-time PCR Assay," *Journal of Water Research*, in prep

SURP RESEARCH PROJECTS — New Initiative — Cognition

Attention in Higher Cognition: Neural Mechanisms

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New Mexico State University

Ann Speed (Org. 6343)
Sandia Principal Investigator

Abstract

The Cognitive Systems group at Sandia has been working to understand the basis of flexible context recognition for a number of years. The current project attempts to develop this understanding at a neurophysiological level through computational modeling of the physiological mechanisms of analogical reasoning. One difficulty with the current neuroimaging literature in analogy, however, is that it reports studies using either functional magnetic resonance imaging (firm) or positron emission tomography (PET), both of which have very nice spatial resolution but poor temporal resolution. Therefore, we have conducted two studies on analogy and prefrontal cortex (PFC) function using electroencephalography (EEG), which provides very nice temporal resolution of cognitive activity. This effort is intended to inform the temporal interactions in different areas of the computational model, which includes representations of cortical function from primary visual cortex through PFC. Specifically, these EEG studies include:

(1) Analogical reasoning - underlying cognitive ability that permits new situations to be understood in terms of existing complex knowledge. Little research has been done to determine the neural mechanisms underlying analogical reasoning. Critical to the project is an understanding of which brain systems are recruited, and how they play a role. Studying the temporal and anatomical nature of brain activity during analogical reasoning will enable us to provide an accurate prescription for how the Cognitive Model should be structured.

(2) Solving problems, or other kinds of higher cognitive processing, requires a sophisticated control of the interaction of top down cognitive control processes, primarily originating from frontal cortex, and bottom up information processing, resulting from perception of information in the world through our perceptual systems. We are using a combination of a high-level task called N-back, with an established study of top-down control of perceptual attention, to determine the configuration and behavior of constituent neural mechanisms participating in mediating simultaneously these two tasks.

These two ongoing projects are funded by Sandia.

Accomplishments

We discovered that frontal cortex is involved in the analogical reasoning task at two critical stages. When mediating problems which require assessing the structural morphology of a problem, an early positive-going component of the ERP waveform (the Evoked Response Potential is a measure of the electrical fields produced by neural responses in the cortex, averaged over several trials, and a component is a particular transient increase in electrical potential—positive or negative—signaling some neural process is occurring) at 200 ms (P2) after stimulus onset appears to correspond to focus of attention or processing resources on the problem, and a later negative-going (processing negativity) at around 600 ms corresponds to the cognitive assessment of structural changes between two stimuli. When no structural change occurred, neither component was present. The components were highly correlated (Pearson's $r > .5$) across cortex. This should eventually inform the cognitive model under development at Sandia.

In a second study, we are observing the interaction between frontal cortex and allotment of attention focus to a problem. This allotment is presumed to be accomplished by frontal regions, but this remains controversial. We ran 10 subjects in an EEG study in which frontal areas are occupied to varying

degrees while an attention task which discriminates automatic attention focusing and conscious, deliberate attention focusing is executed. While participants performed the high-level task as expected, accuracy rates for the attention task were not adequate, even though this task produced reliable results on many previous studies. With pilot work, we determined that the response keys used for the two tasks interfere, and we are running a behavioral pilot to confirm this with new response keys using separate hands for responding to the two tasks.

Publications

J.K. Kroger, A.E. Speed, J.P. Anderson, E.J. Mikkelson, D.K. Spring, and A.L. Polsky. "An ERP Study of Analogical Reasoning," *Psychophysiology*, 44, 2007

J.K. Kroger, A. Speed, E.J. Mikkelsen, J.P. Anderson, A.L. Polsky, and D.K. Spring, "An ERP Study of Relational Complexity in Analogy: Early Gating of Later Processing," to be submitted

The Role of Emotion and Emotion Regulation in Decision Making and Action in Critical Situations

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Abstract

The purpose of this research and development effort is to focus on what is a significant technical gap in existing modeling and simulation capabilities: the representation of trait and state emotion in humans. This proposed effort will provide the empirical data and framework for modeling: (1) the eliciting of strong emotions related to high consequence events (e.g., terrorism, disasters, epidemics), (2) the effect of emotions on the inhibition or facilitation of decision making in these situations, and the (3) the effects of personal characteristics on effective decision making.

Accomplishments

We examined the effects of personal characteristics and emotions on critical decisions in three different samples. The first study was 289 university students responding to an avian flu outbreak scenario. The second study was 259 university students responding to a nuclear explosion scenario. The third study was 82 firefighters responding to the same nuclear explosion scenario.

In Study 1, the personal characteristics studied were resilience and neuroticism, the emotion was negative affect or emotional distress, and the behaviors were economic behaviors including buying essential goods and non-essential and social behaviors including helping, sacrificing, avoidant, and illegal behavior. Neuroticism was related to more distress. Resilience and distress were related to more buying of essential goods and less buying of non-essential goods. Resilience was related to more helping behavior and distress was related to more illegal behavior. Distress was related to more sacrificing for others. Neuroticism and resilience was related to less avoidance and distress to more avoidance.

In Study 2, the personal characteristics studied were resilience, neuroticism, empathy, and a sense of purpose in life, the emotion was emotional distress, and the behaviors were economic behaviors including buying essential goods and non-essential and social behaviors including helping, avoidant, illegal, and destructive behavior. Neuroticism was related to more and resilience to less distress. Purpose in life was related to more and distress to less buying of essential goods. Resilience and neuroticism were related to more buying of non-essential goods. Empathy was related to more and distress to less helping behavior. Distress was related to more and purpose in life to less avoidant behavior. Distress was related to more and neuroticism to less illegal behavior. Purpose in life and empathy were related to less and distress to more destructive behavior.

In Study 3 of the firefighters, the variables were the same as in Study 2. Resilience was related to less and empathy to more distress. Empathy was related to more and neuroticism to less buying of essential goods. Empathy was related to less and distress to more buying of non-essential goods. Empathy was related to more helping and less illegal behavior. Distress and purpose in life were related to more avoidant behavior. Empathy was related to less and purpose in life, resilience, and neuroticism to more destructive behavior.

Thus, our hypothesis that distress would predict behavior was supported for five of six behaviors in Study 1, four of six in Study 2, and three of six in Study 3. In addition, neuroticism was more important than resilience in predicting distress in the avian flu. The main differences between the firefighters and the students were that in the firefighters resilience was a stronger predictor of distress and empathy was related to distress.

Overall, emotional distress was a strong predictor of several important social and economic behaviors during critical situations and should be incorporated into Sandia models of human behavior. In addition, individual differences in

resilience, empathy, and whether people are trained rescue workers or civilians should also be considered in modeling behavior.

Significance

Our work on predicting the emotional and behavioral response to an avian flu outbreak is already in press with the American Journal of Infection Control (see below). The reviewers complimented us on the innovative nature and significance of the work.

We plan to put more emphasis on personal characteristics and individual differences such as resilience and empathy as important factors in understanding the emotional, social, and consumer behavioral responses to critical situations.

We plan to submit a grant to the National Institutes of Health to study resilience and disaster making in citizens and/or first responders to critical incidents. We plan to write a similar additional paper using the data from Study 3 with the firefighters.

Publications

B.W. Smith, V.S. Kay, T.V. Hoyt, and M.L. Bernard, "Predicting the Anticipated Emotional and Behavioral Responses to an Avian Flu Outbreak," *American Journal of Infection Control*, (in press)

B.W. Smith, V.S. Kay, and M.L. Bernard, "Predicting the Anticipated Emotional Distress and Behavior of Citizens Following a Nuclear Explosion Disaster," *Medicine and Public Health Preparedness*, (under review)

SURP RESEARCH PROJECTS — Other: Energy and Environment

Self-sealing Liners for Desalination Evaporation Ponds

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Abstract

The disposal of wastes resulting from desalination processes in evaporation ponds lined with clay-based materials is inexpensive. However, an increase in the concentration of saline wastes due to evaporation reduces the resistance of clay-based lining material to flow, with an apparent decrease in the thickness of the diffuse double layer and an increase in hydraulic conductivity of the lining medium. Consequently, salinity in underlying layers builds up and increases the risk of groundwater pollution. Development of a low-cost, self-healing liner system can minimize the seepage through the bottom of an evaporation pond by precipitating some of the ions and may be a cost-effective solution.

Accomplishments

The objectives presented in the previous report were to: (1) determine the effect of solution electrical conductivity (EC) on the saturated hydraulic conductivity (K_s) and (2) identify a lining material of low K_s that could be used to minimize the leaching of saline wastes from evaporation ponds into the groundwater (Gonzalez et. al., 2007). The objectives in this report were to: (1) study the effect of ponding time of solution on K_s, (2) study the effect of bulk density on the K_s, (3) determine the change in K_s with additional amount of lining material, and (4) evaluate the effect of desiccation of the soil columns on the self-sealing/self-healing capacity of the lining materials.

The materials used in the laboratory experiments were: sodium silicate, magnesium hydroxide, and calcium hydroxide as lining materials, and soil from Tularosa Basin and a surrogate soil. The surrogate soil was composed by crystalline silica (SiO_2), Aluminum Oxide (Al_2O_3), Iron Oxide (Fe_2O_3) and Titanium Oxide (TiO_2). A ratio of 28:78 mass mixture of # 1 dry unground silica and SIL-CO-SIL 125 ground silica was used to replicate the soil from Tularosa. A total of 94 soil columns were used during the entire study, 82 of which were packed with either a layer of lining material sandwiched between soil layers or a homogeneous mix of lining material and soil during the first part of the study. The remaining 12 columns were packed with a layer of lining material during the last part of the study.

The K_s of the surrogate soil without lining material increased with increasing EC. The K_s of the Tularosa soil decreased over time, most likely due to the presence of calcium or magnesium elements in the soil that precipitated after reacting with ions present in the solution. The K_s of the soil and soil-lining material mix increased with increasing EC, but K_s of the layered columns decreased with increasing EC. The reduction of K_s with time indicated that the amount of precipitate formed between the pore spaces increased due to the longer exposure time of the lining material with the ions present in the solution. The results showed that the K_s of the porous medium were inversely

related to the bulk density. The layers of magnesium hydroxide and calcium hydroxide showed self-sealing/self-healing capacity once the dried soil columns were saturated. Both lining materials showed reductions in the K_s of the porous medium and the cracks formed in the soil columns appeared to be sealed. The lowest K_s values before the first desiccation of the soil columns with the calcium hydroxide and magnesium hydroxide were 6.96×10^{-7} m/s and 1.72×10^{-6} m/s, respectively. The lowest K_s values after the third desiccation of the soil columns with the calcium hydroxide and magnesium hydroxide were 4.70×10^{-7} m/s and 1.35×10^{-6} m/s, respectively. The formation of precipitates within the pore spaces has to be evaluated by x-ray diffraction and is currently ongoing at New Mexico State University.

Significance

This study showed that the arrangement of the lining material within the porous medium influenced the K_s. The K_s was lower in columns with layers than columns packed with the homogeneous mix. The layer seemed to provide a larger surface area where the insoluble precipitates were formed. In contrast, lining material in the homogeneous mix did not fill the pore spaces uniformly to slow down the water movement.

Increasing bulk density of the porous medium decreased the K_s. The K_s of porous media decreased with time for all EC's ranging from 0.5 to 30 dS/m. The reduction of K_s with time indicated that the amount of precipitate formed between the pore spaces probably increased due to the increased reaction time between ions in the lining material and the ions present in the solution.

The layers of magnesium hydroxide and calcium hydroxide showed self-sealing and self-healing capacity once the dried soil columns were rewetted. Both lining materials reduced the K_s of the porous medium upon rewetting and the cracks formed in the soil columns were sealed.

The layers of calcium hydroxide and magnesium hydroxide were found to work better than the sodium silicate layer for columns packed with the soil from Tularosa basin. Calcium hydroxide caused maximum reductions in K_s and was identified as the best lining material.

A surrogate soil was included in the study because permission to collect undisturbed and disturbed soil samples from Tularosa Basin Desalination Research Facility was not granted. The study proposed a second bench experiment to test the behavior of the lining materials in undisturbed rectangular soil blocks to be collected from the Tularosa Basin Desalination Research Facility. The undisturbed rectangular soil blocks could not be collected due to the final stage of construction of the Tularosa Basin Desalination Research Facility. Therefore, loose soil samples were collected from a site located close to the Tularosa Basin Desalination Research Facility. These samples were repacked with and without lining materials and were used to conduct additional bench experiments. The initial results showed that the K_s decreased with time. More replicated bench experiments were conducted than proposed in the original proposal, for example, longer duration experiments by repeating the experiments on same columns after a ponding of one day, three days, one week and two weeks after the first conductivity experiments were completed. We also conducted additional experiments using an antiscalant (Nalco Perma Treat PC-19), a chemical compound used in desalination process and is present in the saline wastes, to determine the K_s for layers of calcium hydroxide, magnesium hydroxide and sodium silicate. These experiments were carried out to replicate some of the conditions in the evaporation ponds such as ponding of solution, different bulk densities and desiccation of the porous medium.

The study will be included as a chapter in the A. Gonzalez dissertation that is currently ongoing. However, there is no additional funding available at this time from any agency.

Poster Presentations

A.M. González, S.A. León, M.K. Shukla, and P.V. Brady, "Effect of Solute Concentration on Saturated Hydraulic Conductivity," New Mexico Water Research Symposium, New Mexico Water Resources Research Institute, Socorro, NM, August 14, 2007

A.M. González, M.K. Shukla, and P.V. Brady, "Effect of Electrical Conductivity on the Saturated Hydraulic Conductivity," Joint Meeting (Soil Science Society of America Conference), Houston, TX, October 5 – 9, 2008

Reports

A.M. González, M.K. Shukla, and P.V. Brady, "Self-sealing Liners for Desalination Evaporation Ponds," year-end report of research progress Sandia-University Research Program (SURP) between Sandia National Laboratories and New Mexico State University, 2007

A.M. González, "Effect of Electrical Conductivity on the Saturated Hydraulic Conductivity of Lining Materials," Chapter of PhD Dissertation, Plant and Environmental Science Department, New Mexico State University (Draft: Chapter of PhD Dissertation), 2008

UNIVERSITY OF TEXAS SYSTEM

The University Research Programs Office supports interactions with some universities that do not have "campus executive" status. Such interactions are meant to explore niche technical areas of interest and forge new strategic relationships in critical skills areas. These programs are evaluated regularly to determine their value toward achievement of Sandia's mission objectives.

In FY 2006, Sandia and the University of Texas System (UTS) renewed their commitment to the joint Memorandum of Understanding established in 2005, charging their institutions with strengthening Research Program Interfaces and Collaborations, Peer Review and Scientific Accountability, and Education and Transformation. Their overarching goal is to achieve a greater mutual impact on national security issues. Its strategic purpose is to participate with Sandia scientists on collaborative research projects, to provide peer review for Sandia's research programs, and to provide specialized courses taught by UT professors to increase educational opportunities for Sandians.

Research program interfaces and collaborations in the areas of bioscience and biodefense, healthcare modeling, the National Institute for Nanoengineering (NINE), the National Initiative for Modeling and Simulation (NIMS), and in High Energy Density Physics began in late 2007. Beginning in 2008, potential technical collaborations are being explored in Cognitive Science, and Remote Sensing.

One outcome of the commitment by SNL and UTS is a joint postdoctoral fellowship program across Sandia's Bioscience Research Foundation and UT Medical Branch in Galveston, which began in February 2007. Areas of research being explored include host/pathogen interactions, new bioresearch techniques in microfluidics and other microengineered platforms, advanced imaging, and computational biology. This program is rapidly growing the Research Program Interfaces across the two institutions and will serve as the springboard for building future programs.

UTS is providing independent oversight to assess and enhance Sandia's Science, Technology and Engineering excellence through the Peer Review process. Beginning in 2007, at the request of the Science and Technology Subcommittee of the Missions Committee of the Sandia Board of Directors, the UTS Vice Chancellor for Research and Technology Transfer assumed responsibility for decisions associated with the membership of the six Research Foundation External Review Panels (ERPs). Chairs of each ERP also serve as members of the Sandia Science Advisory Board (SSAB). Working in concert with the Sandia Chief Technology Officer, formal, independent UTS oversight of the panel vetting process continues to be critical to the integrity of the external advisory and review process.

The partnership in Education has directly benefited Sandians. The Texas State legislature, in 2005, granted the UT System permission to charge in-state tuition and fees to employees and dependents of organizations working with UT in science and technology development. Sandians and their dependents can pay in-state rates when enrolled at a University of Texas System institution. This benefit also extends to those taking distance-learning classes. In FY2008, the groundwork was laid for the first technical education series – a 15-week seminar course in Discrete Element Modeling of Particle Systems which was jointly designed by UT faculty and Sandia staff.

Sandia has had memoranda of understanding with UT Austin for approximately seven years and with UT El Paso for nine years. Various research projects have been ongoing. As a result of the emphasis on new collaborations, at least 32 research projects exist. This number includes 7 new projects at UT Medical Branch, Galveston, up from 3 last year.

In FY08, Sandia had research contracts totaling $1.7 million with UT Austin, UT El Paso, and UT Medical Branch. There were no contracts placed with UT Arlington, Dallas, or Southwestern Medical Center. Approximately 192 UT System graduates are currently employed at Sandia, up from 156 in FY07. In addition, 9 students from the UT System currently work for Sandia.